

Sufficient conditions for absolute convergence of hardcore cluster expansions

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Abstract

We present several new sufficient conditions for uniform boundedness of the reduced correlations and free energy of an abstract polymer system in a small complex disc around zero fugacity. In particular, we solve a discrepancy between several known conditions, which are not always comparable, and show how they arise from a common approach. The main tool is an extension of the tree-operator approach introduced by Fernández & Procacci combined with novel partition schemes of the spanning subgraph complex of a cluster.

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1 Introduction

A recurring theme in statistical mechanics is the search for improved lower bounds of the radius of analyticity of the cluster expansion of an abstract polymer system around zero fugacity. This usually demands a convergence argument and a sufficient condition for uniform boundedness (short SCUB) of finite volume quantities.

The first such SCUBs have been derived by Gruber & Kunz [GK71], still in the context of subset polymer systems, and Kotecký & Preiss [KP86]. Both are based on cluster expansion techniques. A major improvement, in particular because of its short proof, has been Dobrushin's SCUB [Dob96a]. It first bounds the reduced correlations, that is ratios of partition functions, which entails the boundedness of the free energy.

Recent work by Fernández & Procacci [FP07] uses an identity by Penrose [Pen67] to convert the problem of bounding the cluster expansion to determining a non-trivial fixpoint of a tree-operator. Their SCUB improves on Dobrushin's SCUB by not only accounting for the number of polymers incompatible with each polymer, but also their mutual incompatibilities. They also show that all

the previously known SCUBs are reproducible within their framework of tree-operators and are relaxations of their SCUB.

There is another Dobrushin-style SCUB building on work of Liggett, Schonmann & Stacey [LSS97] and Scott & Sokal [SS05], which reduces the degree of Dobrushin's SCUB by one. On locally tree-like graphs it is better than Fernández & Procacci's SCUB. This discrepancy has been the main motivation in our search for an interpretation the above reduced-degree SCUB in the context of tree-operators, its improvement and the clarification of its relation with the other SCUBs.

This paper presents several new SCUBs of increasing strength and complexity. We show that all new and known SCUBs arise in a generalised tree-operator framework and are specialisations of a single, stronger SCUB. The novel mathematical techniques are threefold: First, a generic relaxation transforming weaker SCUBs into the ones we want. Second, explorative partition schemes, which allow for tighter tree approximations via Penrose's theorem by keeping more restrictions on trees exploitable by the tree-operator framework. Third, multiplexing bounds onto spaces indexed by more information than just the set of polymers, which allows restrictions on trees to be carried over between successive applications of the tree-operators.

Via the explicit connection between the Lovász Local Lemma and the partition function of the abstract polymer system at negative real fugacity made by Scott & Sokal [SS05], the new SCUBs are improvements of the Lovász Local Lemma.

The organisation of this paper is as follows: In the following subsections we introduce notation, key quantities and basic identities. Section 2 lists all known SCUBs in order of increasing strength and discusses the results. Section 3 rassembles all the Dobrushin-style inductive proofs. Section 4 introduces the tree-operator framework and section 5 explorative partition schemes, which section 6 combines into the proof of the SCUBs.

1.1 Setup and notation

We have a countable set of polymers \mathcal{P} with a symmetric and reflexive incompatibility relation \approx (we choose \approx instead of $\not\approx$ to mimic the standard graph theoretic notation for adjacency in the induced graph (\mathcal{P}, \approx)). Without loss of generality, we assume that the graph (\mathcal{P}, \approx) is connected and locally finite. For each polymer γ , we write $\mathcal{I}(\gamma)$ for the set of polymers incompatible with γ and $\mathcal{I}^*(\gamma) := \mathcal{I}(\gamma) \setminus \{\gamma\}$ for the set of polymers incompatible with and different than γ .

For every finite subset of polymers $\Lambda \in \mathcal{P}$, we define the *grand canonical partition function* $\Xi_\Lambda : \mathbb{C}^\Lambda \rightarrow \mathbb{C}$ by

$$\Xi_\Lambda(\vec{z}) := \sum_{\text{compatible}} \prod_{I \subseteq \Lambda} z_I \quad (1a)$$

$$= \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in \Lambda^n} \left(\prod_{1 \leq i < j \leq n} [\xi_i \not\approx \xi_j] \right) \prod_{i=1}^n z_{\xi_i}. \quad (1b)$$

where \vec{z} are the *activities* or *fugacities* on Λ . It follows that $\Xi_\emptyset(\vec{z}) = 1$. The function $\Xi_\Lambda(\vec{z})$ is affine in each parameter z_γ .

Scalar arithmetic operations and comparisons are lifted component-wise to vectors. The *projection* of a vector $\vec{x} := (x_\gamma)_{\gamma \in \mathcal{P}}$ to a subset $\Lambda \subseteq \mathcal{P}$ is \vec{x}_Λ , if needed for disambiguation, otherwise silently ignoring superfluous coordinates.

1.2 Key quantities and identities

This section states the key quantities of interest and relations between them. Every definition and relation is a priori just formal, as not all the divisions are well-defined for all complex \vec{z} . They are well-defined though, if one of the SCUBs is satisfied. There are two principal quantities of interest. The first is the *reduced correlation* [GK71] of m distinct polymers ξ_1, \dots, ξ_m

$$\Phi_\Lambda^{\xi_1, \dots, \xi_m}(\vec{z}) := \frac{\Xi_{\Lambda \setminus \bigcup_{i=1}^m \mathcal{I}(\xi_i)}(\vec{z})}{\Xi_\Lambda(\vec{z})}. \quad (2a)$$

The second is the *free energy*

$$F_\Lambda(\vec{z}) := -\frac{\log \Xi_\Lambda(\vec{z})}{|\Lambda|}. \quad (2b)$$

The aim is to find bounds on these quantities independently of Λ , that is in the *thermodynamic limit*. From here on we assume that $\gamma \in \Lambda$. Secondary quantities also of interest are the *pinned connected function* [Far10, (2.24)]

$$\frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(\vec{z}) \quad (2c)$$

and the *rooted connected function* [Far10, (2.25)]

$$z_\gamma \frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(\vec{z}). \quad (2d)$$

Again we want bounds uniformly in Λ . We introduce the *one polymer partition ratios*

$$\varphi_\Lambda^\gamma(\vec{z}) := \frac{\Xi_\Lambda(\vec{z})}{\Xi_{\Lambda \setminus \{\gamma\}}(\vec{z})}. \quad (3)$$

For $\{\xi_1, \dots, \xi_n\} := \Lambda \subseteq \mathcal{P}$ and $\Lambda_i := \{\xi_1, \dots, \xi_i\}$, the *telescoping identity* expresses the partition function as a product of one polymer partition ratios:

$$\Xi_\Lambda(\vec{z}) = \prod_{i=1}^n \varphi_{\Lambda_i}^{\xi_i}(\vec{z}). \quad (4)$$

Similarly, each reduced correlation is a products of inverses of suitable chosen one polymer partition ratios. Also, the pinned connected function is a product of reduced correlations [SS05, (3.8)] and the logarithm of the reduced correlations is an integral over the pinned connected function [BFPS11, (A.3)]. See section 10 for further details.

1.3 Cluster expansion and the worst case

Let I be a finite set. A vector $\vec{\xi} := (\xi_i)_{i \in I} \in \mathcal{P}^I$ has *support*

$$\text{supp } \vec{\xi} := \{\gamma \in \mathcal{P} : \exists i \in I : \xi_i = \gamma\}. \quad (5)$$

The vector $\vec{\xi}$ *induces* the graph

$$G(\vec{\xi}) := (I, \{(i, j) \in I^2 : \xi_i \approx \xi_j\}). \quad (6)$$

If this graph is connected, then it is called a *cluster*. A classic approach is to rewrite the logarithm of the partition function via the *cluster expansion* [MS10], [Far10, section 2.5], [SS05, section 2.2]. Define the *Ursell functions* [Urs27] (or *semi-invariants* [Dob96a] or *truncated functions* [SS05]) as

$$u(\vec{\xi}) := \begin{cases} 1 & |I| = 1, \\ \sum_{H \in \mathcal{C}_{G(\vec{\xi})}} (-1)^{|E(H)|} & |I| \geq 2 \text{ and } G(\vec{\xi}) \text{ connected,} \\ 0 & \text{else.} \end{cases} \quad (7)$$

The *spanning subgraph complex* \mathcal{C}_G of a graph G is introduced in section 4.1. We formally expand the logarithm of the partition function to

$$\log \Xi_\Lambda(\vec{z}) \stackrel{F}{=} \sum_{n \geq 1} \frac{1}{n!} \sum_{\vec{\xi} \in \Lambda^n} u(\vec{\xi}) \prod_{i=1}^n z_{\xi_i}. \quad (8)$$

The expansion of the pinned connected function is consequently

$$\frac{\partial \log \Xi_\Lambda(\vec{z})}{\partial z_\gamma} \stackrel{F}{=} \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in \{\gamma\} \times \Lambda^n} u(\vec{\xi}) \prod_{i=1}^n z_{\xi_i} \quad (9)$$

The *Ursell functions* have the *alternating sign property* [SS05, proposition 2.8]

$$(-1)^{|I|+1} u(\vec{\xi}) \geq 0. \quad (10)$$

This implies that the worst case is for negative real fugacities:

$$\left| \frac{\partial \log \Xi_\Lambda(\vec{z})}{\partial z_\gamma} \right| \leq \frac{\partial \log \Xi_\Lambda(-|\vec{z}|)}{\partial z_\gamma} \quad \text{and} \quad \varphi_\Lambda^\gamma(-|\vec{z}|) \leq |\varphi_\Lambda^\gamma(\vec{z})|. \quad (11)$$

2 Sufficient conditions for uniform boundedness

This paper is about sufficient conditions for uniform boundedness (short SCUB) of the quantities (2) around $\vec{0}$ fugacity. A SCUB implies uniform (in Λ) bounds of either the form

$$\exists \vec{C} \in]0, \infty[^{\mathcal{P}} : \forall \gamma \in \Lambda \in \mathcal{P} : \frac{\partial \log \Xi_\Lambda(-|\vec{z}|)}{\partial z_\gamma} \leq C_\gamma \quad (12a)$$

or

$$\exists \vec{c} \in]0, \infty[^{\mathcal{P}} : \forall \gamma \in \Lambda \in \mathcal{P} : c_\gamma \leq \varphi_\Lambda^\gamma(-|\vec{z}|). \quad (12b)$$

As we can express the pinned connected expression in the one polymer partition ratios (66) and vice-versa (67), the bounds in (12) are equivalent. If a SCUB is satisfied for some $\vec{\rho}$, then all the definitions and relations in sections 1.2 and 1.3 are well-defined for every complex \vec{z} with $|\vec{z}| \leq \vec{\rho}$ [SS05, theorem 2.10].

The uniform boundedness is equivalent to the well-definedness and non-negativity of the following quantity:

$$\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) := \lim_{\Lambda \nearrow \mathcal{P}} \varphi_{\Lambda}^{\gamma}(-\vec{\rho}), \quad (13)$$

where the limit is monotone decreasing [SS05, top of page 62] in the ultra-filter of finite subsets of \mathcal{P} containing γ .

2.1 Admissible parameters

As we primarily care about negative real fugacities, we introduce the *multidisc of admissible parameters*

$$\mathcal{R}_{\mathcal{P}} := \{ \vec{\rho} \in [0, \infty[^{\mathcal{P}} : \quad \forall \Lambda \in \mathcal{P} : \quad \Xi_{\Lambda}(-\vec{\rho}) > 0 \}. \quad (14)$$

The set $\mathcal{R}_{\mathcal{P}}$ is an intersection of open sets and almost closed [SS05, theorem 8.1]. The *interior* of $\mathcal{R}_{\mathcal{P}}$, with respect to the *box-topology*, is

$$\text{Int } \mathcal{R}_{\mathcal{P}} := \{ \vec{\rho} \in \mathcal{R}_{\mathcal{P}} : \quad \exists \vec{x} > \vec{0} : \quad \vec{\rho} + \vec{x} \in \mathcal{R}_{\mathcal{P}} \}, \quad (15)$$

Both $\mathcal{R}_{\mathcal{P}}$ and $\text{Int } \mathcal{R}_{\mathcal{P}}$ are *log-convex* and a *down-set* [SS05, proposition 2.5], i.e., if $\vec{\rho} \in \mathcal{R}_{\mathcal{P}}$, then every $\vec{\mu}$ with $\vec{0} \leq \vec{\mu} \leq \vec{\rho}$ is also in $\mathcal{R}_{\mathcal{P}}$. Proposition 1 shows a generic SCUB based on $\text{Int } \mathcal{R}_{\mathcal{P}}$.

Proposition 1. *If $\vec{0} \leq \vec{\rho} \leq \vec{\mu} \in \mathcal{R}_{\mathcal{P}}$, then*

$$\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) \geq \begin{cases} \frac{\mu_{\gamma} - \rho_{\gamma}}{\mu_{\gamma}} & \text{if } \mu_{\gamma} > 0 \\ 1 & \text{if } \mu_{\gamma} = 0. \end{cases} \quad (16)$$

In particular, we have

$$\vec{\rho} \in \text{Int } \mathcal{R}_{\mathcal{P}} \Rightarrow (\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) > 0). \quad (17)$$

Its proof is in section 3. Proposition 1 is inspired by a coupling [Tem12, model 22] in the context of the interpretation as Shearer's measure [She85, SS05]. The importance of proposition 1 lies in the the ability to lift a weaker SCUB, which just guarantees $\vec{\rho}$ to lie in $\mathcal{R}_{\mathcal{P}}$, to a SCUB in our sense, by slightly relaxing it by restriction to $\text{Int } \mathcal{R}_{\mathcal{P}}$.

Example 7 shows that at least in one case analyticity breaks down at a boundary point of $\mathcal{R}_{\mathcal{P}}$. This is shown by the infinite-volume limit of the one-polymer ratios at that boundary point. As we believe that this break-down holds all along the boundary, a SCUB should only ever map out subsets of the $\text{Int } \mathcal{R}_{\mathcal{P}}$. Thus our search for SCUBs can be reformulated as:

Question 2. What are the properties of $\mathcal{R}_{\mathcal{P}}$? What are sufficient (or necessary) conditions for $\vec{\rho}$ to be in $\mathcal{R}_{\mathcal{P}}$?

We point out that there has been work [SS05, section 8.2] on necessary conditions, too. Necessary conditions correspond to supersets of $\mathcal{R}_{\mathcal{P}}$.

2.2 Discrepancy in the homogeneous case

The setting for this section is: (\mathcal{P}, \approx) is a transitive graph of *degree* $D := |\mathcal{I}^*(\gamma)|$ (ignoring the loops in (\mathcal{P}, \approx)) and we have homogeneous fugacity $z\bar{1}$. The motivation of our paper stems from the comparison of various SCUBs in the literature, in this setting.

The classic SCUB by Dobrushin [Dob96b], also known as the *symmetric Lovász Local Lemma* [EL75], is

$$\rho \leq \sup_{\mu > 0} \frac{\mu}{(1 + \mu)^{D+1}} = \frac{D^D}{(D + 1)^{(D+1)}}. \quad (18a)$$

An improved SCUB by Fernández & Procacci [FP07] is

$$\rho \leq \sup_{\mu > 0} \frac{\mu}{\Xi_{\mathcal{I}(\gamma)}(\mu)}. \quad (18b)$$

If (\mathcal{P}, \approx) is *triangle-free*, that is the subgraph $(\mathcal{I}(\gamma), \approx)$ is a star, for every $\gamma \in \mathcal{P}$, then (18b) reduces to (18a). Both of these SCUBs have interpretations as tree-operators in the framework by Fernández & Procacci. There is another SCUB, though, independently discovered by [LSS97] and [SS05], namely

$$\rho < \sup_{\mu > 0} \frac{\mu}{(1 + \mu)^D} = \frac{(D - 1)^{(D-1)}}{D^D}. \quad (18c)$$

The improvement over (18a) is the reduction of the degree by one. The reason for the strict inequality in (18c) is a hidden application of proposition 1 (see the proof of (22) in section 3). The SCUB (18c) is exact on D -regular infinite trees under homogeneous fugacity [She85]. In this case (18c) is stronger than (18b), while it is weaker in other cases. The following questions arose from this discrepancy:

Question 3. Is there a tree-operator hidden behind (18c), too?

Question 4. Can we improve (18c) in a similar way as (18b) improved on (18)?

Question 5. Is there a unified approach towards all of these SCUBs? Can it unite (18b) and a possible improvement from question 4?

Section 2.3 affirmatively answers these three questions.

2.3 Main results

This section presents the new SCUBs, answers our questions and compares them to the known ones. The relationship is summarised in figure 1. We give an intuitive back-of-the-envelope graphical explanation in terms of counting tree extensions of depth 1 in section 2.4.

We recall the known SCUBs by Kotecký & Preiss (20a) [KP86], Dobrushin (20b) [Dob96b] and Fernández & Procacci (20c) [FP07]. They have the form: if there exist $\vec{\rho}, \vec{\mu} \in [0, \infty]^{\mathcal{P}}$, such that

$$\vec{\rho} \phi^{\text{gen}}(\vec{\mu}) \leq \vec{\mu} \Rightarrow \left(\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) > 0 \right), \quad (19)$$

where $\phi^{\text{gen}} : [0, \infty]^{\mathcal{P}} \rightarrow [0, \infty]^{\mathcal{P}}$ is particular to each SCUB. The SCUBs are, in order and for each γ :

$$\phi_{\gamma}^{\text{KP}}(\vec{\mu}) := \exp \left(\sum_{\xi \in \mathcal{I}(\gamma)} \mu_{\xi} \right) \quad (20a)$$

$$\phi_{\gamma}^{\text{Dob}}(\vec{\mu}) := \prod_{\xi \in \mathcal{I}(\gamma)} (1 + \mu_{\xi}) \quad (20b)$$

$$\phi_{\gamma}^{\text{FP}}(\vec{\mu}) := \Xi_{\mathcal{I}(\gamma)}(\vec{\mu}). \quad (20c)$$

Dobrushin's SCUB (20b) is also known as the *asymmetric Lovász Local Lemma* [EL75].

The new SCUBs have the form: if there exist $\vec{\rho}, \vec{\mu} \in [0, \infty]^{\mathcal{P}}$, such that

$$\vec{\rho} \phi^{\text{gen}}(\vec{\mu}) < \vec{\mu} \Rightarrow (\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) > 0), \quad (21)$$

where $\phi^{\text{gen}} : [0, \infty]^{\mathcal{P}} \rightarrow [0, \infty]^{\mathcal{P}}$ is a particular to each SCUB. The reason for the strict inequality is an application of proposition 1, as our SCUBs directly only imply that $\vec{\rho} \in \mathcal{R}_{\mathcal{P}}$. Our first SCUB is a *reduced degree* version of Dobrushin's SCUB (20b) and the inhomogeneous version of (18c):

$$\phi_{\gamma}^{\text{red}}(\vec{\mu}) := (1 + \mu_{\gamma}) \max_{\varepsilon \in \mathcal{I}^*(\gamma)} \prod_{\xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}} (1 + \mu_{\xi}). \quad (22)$$

Its proof is in section 3: it is a short induction á la Dobrushin, avoiding cluster expansion. Knowing Fernández & Procacci's tree-operators, question 3 arises immediately: does $\vec{\rho} \phi^{\text{red}}(\vec{\mu})$ correspond to a yet unknown tree-operator? It is so, and the improvement, analogously to ϕ^{FP} improving upon ϕ^{Dob} , is the *returning* SCUB

$$\phi_{\gamma}^{\text{ret}}(\vec{\mu}) := (1 + \mu_{\gamma}) \max_{\varepsilon \in \mathcal{I}^*(\gamma)} \Xi_{\mathcal{I}^*(\gamma) \setminus \{\varepsilon\}}. \quad (23)$$

The naming is explained in section 2.4 and the proof is in section 6.1. While ϕ^{ret} improves ϕ^{red} , it is still not comparable with ϕ^{FP} . There is generalisation of them both, though. Define the *set of compatible polymer pairs* as

$$\mathcal{P}_{\star} := \{(\gamma, \varepsilon) : \gamma \in \mathcal{P}, \varepsilon \in \mathcal{I}^*(\gamma)\}. \quad (24)$$

For $\vec{g} \in \{\mathbf{G}, \mathbf{R}\}^{\mathcal{P}_{\star}}$, let

$$\forall \varepsilon \in \mathcal{P} \quad G_{\varepsilon}^{\text{out}(\vec{g})} := \{\gamma \in \mathcal{I}^*(\varepsilon) : \quad b_{(\gamma, \varepsilon)} = \mathbf{G}\}, \quad (25a)$$

$$\forall \gamma \in \mathcal{P} \quad G_{\gamma}^{\text{in}(\vec{g})} := \{\varepsilon \in \mathcal{I}^*(\gamma) : \quad b_{(\gamma, \varepsilon)} = \mathbf{G}\}. \quad (25b)$$

The *synthetic* SCUB at $\vec{g} \in \{\mathbf{G}, \mathbf{R}\}^{\mathcal{P}_{\star}}$ is

$$\begin{aligned} \phi_{\gamma}^{\text{syn}(\vec{g})}(\vec{\mu}) := \max \Big\{ & \Xi_{G_{\gamma}^{\text{out}(\vec{g})}}(\vec{\mu}) \Xi_{\mathcal{I}(\gamma) \setminus G_{\gamma}^{\text{out}(\vec{g})}}(\vec{\mu}), \\ & (1 + \mu_{\gamma}) \max_{\varepsilon \in G_{\gamma}^{\text{in}(\vec{g})}} \Xi_{G_{\gamma}^{\text{out}(\vec{g})} \setminus \{\varepsilon\}}(\vec{\mu}) \Xi_{\mathcal{I}^*(\gamma) \setminus G_{\gamma}^{\text{out}(\vec{g})} \setminus \{\varepsilon\}}(\vec{\mu}) \Big\}. \end{aligned} \quad (26)$$

Finally, the *synthetic* SCUB, for $\vec{\rho}$, has its own form. It is the supremum over all choices of \vec{g} :

$$\begin{aligned} & \left(\exists \vec{g} \in \{0, 1\}^{\mathcal{P}}, \exists \vec{\mu} \in [0, \infty[^{\mathcal{P}} : \forall \gamma \in \mathcal{P} : \quad \vec{\rho} \phi_{\gamma}^{\text{syn}(\vec{g})}(\vec{\mu}) < \vec{\mu} \right) \\ & \Rightarrow \left(\forall \gamma \in \mathcal{P} : \quad \varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) > 0 \right). \end{aligned} \quad (27)$$

The expression $\phi_{\gamma}^{\text{syn}(\vec{g})}$ reduces to $\phi_{\gamma}^{\text{FP}}$ and $\phi_{\gamma}^{\text{ret}}$, for particular choices of \vec{g} :

$$\phi_{\gamma}^{\text{FP}} = \phi_{\gamma}^{\text{syn}(\vec{\mathbf{G}})} \quad \text{and} \quad \phi_{\gamma}^{\text{ret}} = \phi_{\gamma}^{\text{syn}(\vec{\mathbf{R}})}. \quad (28)$$

The vector \vec{g} interpolates between the behaviour of ϕ^{Dob} and ϕ^{FP} . In the homogeneous (both in (\mathcal{P}, \approx) and $\vec{\rho}$) setting of section 2.2, $\phi_{\gamma}^{\text{syn}(\vec{g})}$ reduces to exactly one of (20c) and (23).

The domains of $\vec{\rho}$, for which the SCUBs (22), (23) and (27) hold, are log-convex and down-sets. A direct proof follows from the arguments in [FP07, proposition 3], while a generic argument follows from [SS05, proposition 2.15].

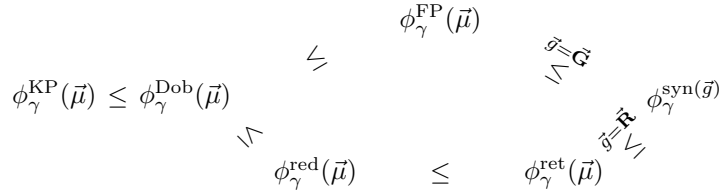


Figure 1: Relationship between the SCUBs

2.4 Graphical explanation

At this point we have mentioned tree-operators, but not told yet what they really are. While we leave the formal definition to section 4, we want to give a back-of-the-envelope explanation here. The key part of the proof of each SCUB is the convergence of a series over weighted, labelled and rooted trees. The labels are polymers attached to the vertices of the tree and determine the weight. A tree-operator builds these trees in an iterative fashion and thus control the convergence of the resulting series. A depth 1 tree-operator, applied at some depth n , takes a labelled tree of depth n and produces several new trees, with corresponding weights, from it. It does so by replacing the weight of the leaf by the corresponding entry of $\vec{\rho}$ and adding a finite, but possibly zero, number of children. The children get weights drawn from μ . This happens independently for each level n leaf of the original tree.

We want to explain this by a concrete example. In figure 2 you find the graph of the incompatible neighbourhood of the polymer γ . Suppose we are at a level n leaf v of a depth n tree, labelled by γ . The possible labels of children of v have to come from $\mathcal{I}(\gamma)$, due to the structure of a cluster (see figure 5). The different SCUBs stem from different tree-operators, which differ in the labels they allow for the children of v .

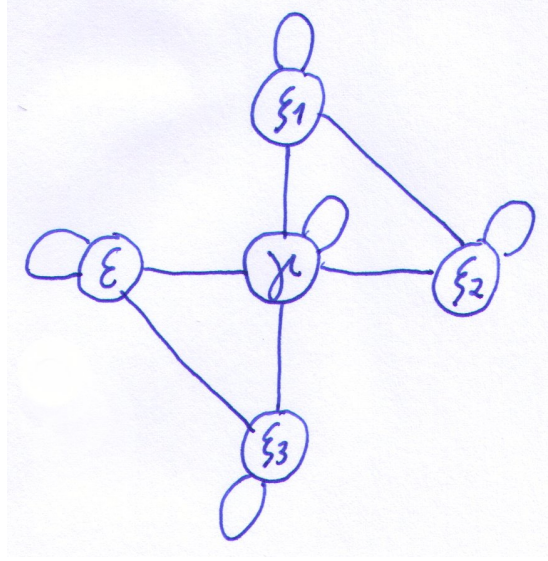


Figure 2: The example polymer incompatible neighbourhood graph $(\mathcal{I}(\gamma), \approx)$ we use in our graphical explanation. Lines represent incompatibilities. Recall that each polymer is incompatible with itself.

In figure 3 we describe the different tree-operators by listing the constraints on the labels of possible children of v , which carries label γ . The notation is: thick lines are incompatibilities between the labels of the children taken into account, thin lines are ignored incompatibilities and crossed out polymers are ignored.

The first figure 3(a) describes Kotecký & Preiss's ϕ^{KP} operator: all incompatibilities are ignored. Thus there is a finite number of children for each polymer incompatible with γ , leading to a $\exp(\mu_\xi)$ factor, for each $\xi \in \{\gamma, \xi_1, \xi_2, \xi_3, \varepsilon\}$, and subsequently their product in (20a). This tree-operator assumes nothing else than the structure of (\mathcal{P}, \approx) .

Dobrushin's and Fernández & Procacci's SCUBs are drawn in figures 3(b) and 3(c) respectively. Here we encounter the first red lines, which mark incompatibilities taken into account. In the case of Dobrushin's SCUB these are only the loops. This translates into the restriction: at most one child labelled by each polymer. Thus a $(1 + \mu_\xi)$ factor, for each $\xi \in \{\gamma, \xi_1, \xi_2, \xi_3, \varepsilon\}$, and subsequently their product in (20b). Fernández & Procacci's SCUB takes into account also the incompatibilities between the polymers. Thus the polymer labels of each possible extension of a leaf must form an independent subset of $(\{\gamma, \xi_1, \xi_2, \xi_3, \varepsilon\} = \mathcal{I}(\gamma), \approx)$. Summing these up yields $\Xi_{\mathcal{I}(\gamma)}(\vec{\mu})$.

The final two figures describe the new reduced and returning SCUBs. There the polymer ε has another interpretation. It marks the last polymer label different to γ on the path from the root of the tree to the leaf (admitting momentarily, that such a different label exists). The tree-operator disallows returning to this

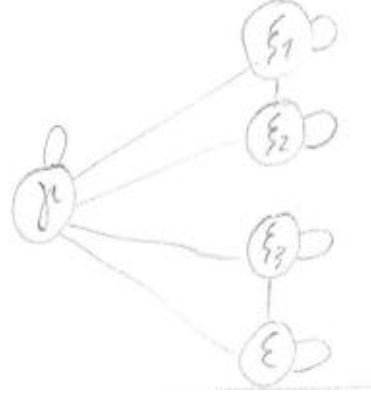
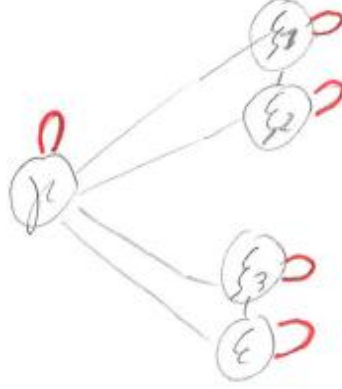
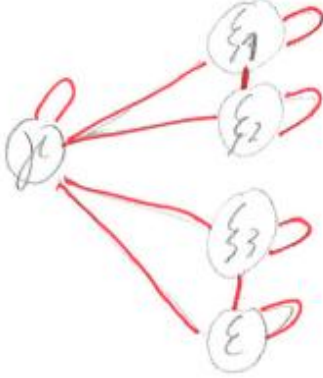
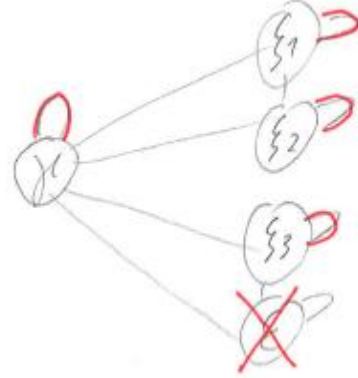
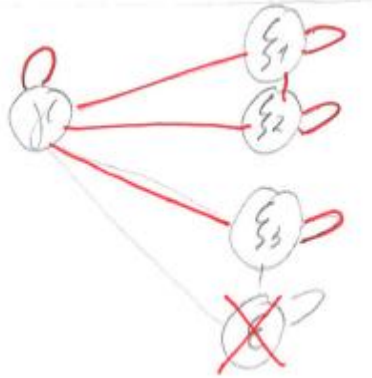
(a) Graphical explanation of $\phi_\gamma^{\text{KP}}(\vec{\mu})$ (b) Graphical explanation of $\phi_\gamma^{\text{Dob}}(\vec{\mu})$ (c) Graphical explanation of $\phi_\gamma^{\text{FP}}(\vec{\mu})$ (d) Graphical explanation of $\phi_\gamma^{\text{red}}(\vec{\mu})$ (e) Graphical explanation of $\phi_\gamma^{\text{ret}}(\vec{\mu})$

Figure 3: Graphical explanation of the SCUBs by counting depth 1 trees, based on the example in figure 2. The incompatibilities are marked in either red or blue. The incompatibilities in red are taking into account. In figures (e) and (d) the stroken-through ε is the last different ancestor polymer and thus ignored.

last visited polymer label. The price for this ignorance of incompatibilities between γ and $\{\xi_1, \xi_2, \xi_3, \varepsilon\}$, leading to the separate $(1 + \mu_\gamma)$ factor in both (22) and (23).

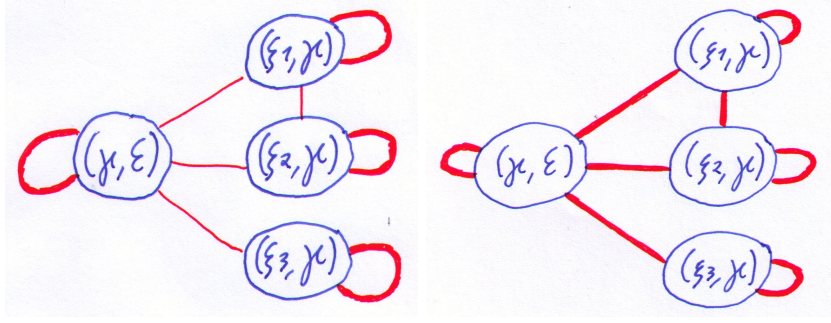


Figure 4: Graphical explanation on extended directed polymer system. Above you see, for ϕ_γ^{red} on the left side and ϕ_γ^{ret} on the right side, the possible labels of the children of a vertex with label (γ, ε) in the corresponding term of the max. The lines show the incompatibilities and thick lines are the incompatibilities taken into account, based on the example in figure 2.

In fact, both tree-operators act on a space indexed by \mathcal{P}_\star from (24). This is necessary to carry the information about the last different polymer label between successive applications of the tree-operator. See the graphical representation in figure 4. For the details see section 6.1. The tree-operator behind the synthetic SCUB is not explained, as its behaviour interpolates between the reduced and returning behaviour, depending on \vec{g} and possibly different at each polymer.

3 Polymer level inductive proofs

This section contains the polymer level inductive proofs, i.e. proofs using the *deletion-contraction properties* of the partition function instead of cluster expansion. The key is the *fundamental identity*:

$$\forall \gamma \in \Lambda \in \mathcal{P} : \quad \Xi_\Lambda(\vec{z}) = \Xi_{\Lambda \setminus \{\gamma\}}(\vec{z}) + z_\gamma \Xi_{\Lambda \setminus \mathcal{I}(\gamma)}(\vec{z}). \quad (29a)$$

In terms of the one polymer partition ratios, and if $\Xi_{\Lambda \setminus \{\gamma\}}(\vec{z}) \neq 0$, it becomes

$$\varphi_\Lambda^\gamma(\vec{z}) = 1 + \frac{z_\gamma}{\prod_{i=1}^m \varphi_{\Lambda \setminus \{\gamma, \xi_{i+1}, \dots, \xi_m\}}^{\xi_i}(\vec{z})}, \quad (29b)$$

where $\{\xi_1, \dots, \xi_m\} := \mathcal{I}^*(\gamma) \cap \Lambda$. We recall the monotonicity properties of the one polymer partition ratios:

Lemma 6 ([SS05, top of page 62], [Tem12, (5.67)]). *For $\gamma \in \Lambda \in \mathcal{P}$, if $\Xi_{\Lambda \setminus \{\gamma\}}(-\vec{\rho}) > 0$, then*

$$\forall \Lambda' \subseteq \Lambda : \quad \varphi_{\Lambda'}^\gamma(-\vec{\rho}) \leq \varphi_\Lambda^\gamma(-\vec{\rho}), \quad (30a)$$

$$\forall \vec{0} \leq \vec{\mu} \leq \vec{\rho} : \quad \varphi_\Lambda^\gamma(-\vec{\rho}) \leq \varphi_\Lambda^\gamma(-\vec{\mu}). \quad (30b)$$

That is, the one polymer partition ratios are decreasing in both volume and negative fugacity. Equations (30b) and (4) together imply that $\mathcal{R}_{\mathcal{P}}$ is a down-set.

Proof of proposition 1. We prove the bound (17), for all $\gamma \in \Lambda \in \mathcal{P}$, by induction over the cardinality of Λ and then take the limit $\Lambda \nearrow \mathcal{P}$. If $\mu_{\gamma} = 0$, then $0 \leq \rho_{\gamma} \leq \mu_{\gamma} = 0$ and $\varphi_{\Lambda}^{\gamma}(-\vec{\rho}) = 1 - \rho_{\gamma} = 1$, independent of the cardinality of Λ . We therefore assume that $\vec{\rho} > \vec{0}$ for the remainder of this proof. The induction base with $\Lambda = \{\gamma\}$ is given by

$$\varphi_{\{\gamma\}}^{\gamma}(-\vec{\rho}) = 1 - \rho_{\gamma} \geq 1 - \frac{\rho_{\gamma}}{\mu_{\gamma}} = \frac{\mu_{\gamma} - \rho_{\gamma}}{\mu_{\gamma}}.$$

For the induction step let $\{\xi_1, \dots, \xi_m\} := \mathcal{I}^*(\gamma) \cap \Lambda$. Then

$$\begin{aligned} & \varphi_{\Lambda}^{\gamma}(-\vec{\mu}) \\ &= 1 - \frac{\mu_{\gamma}}{\prod_{i=1}^m \varphi_{\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}}^{\xi_i}(-\vec{\mu})} && \text{by (29b)} \\ &= 1 - \frac{\mu_{\gamma}}{\rho_{\gamma}} \frac{\rho_{\gamma}}{\prod_{i=1}^m \varphi_{\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}}^{\xi_i}(-\vec{\mu})} && \text{we assume } \rho_{\gamma} > 0 \\ &\geq 1 - \frac{\mu_{\gamma}}{\rho_{\gamma}} \frac{\rho_{\gamma}}{\prod_{i=1}^m \varphi_{\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}}^{\xi_i}(-\vec{\rho})} && \text{as } \vec{\rho} \leq \vec{\mu} \text{ and by (30b)} \\ &\geq 1 - \frac{\mu_{\gamma}}{\rho_{\gamma}} (1 - \varphi_{\Lambda}^{\gamma}(-\vec{\rho})) && \text{by (29b)} \end{aligned}$$

Therefore

$$\varphi_{\Lambda}^{\gamma}(-\vec{\rho}) \geq \frac{\mu_{\gamma} - \rho_{\gamma}}{\mu_{\gamma}} + \frac{\rho_{\gamma}}{\mu_{\gamma}} \varphi_{\Lambda}^{\gamma}(-\vec{\mu}) \geq \frac{\mu_{\gamma} - \rho_{\gamma}}{\mu_{\gamma}}.$$

□

Proof of (22). The first part of this proof shows that uniform bounds on a certain subclass of the one polymer partition ratios are already sufficient, while the second part gives such a bound.

We say that a one polymer partition ratio, identified with (Λ, γ) , is *escaping* iff $\mathcal{I}^*(\gamma) \setminus \Lambda \neq \emptyset$. If (Λ, γ) is escaping, then every polymer in $\mathcal{I}^*(\gamma) \setminus \Lambda$ is an *escape* of (Λ, γ) . Suppose we have, for $\vec{\rho} \geq \vec{0}$, a uniform bound on escaping one polymer partition ratios. That is, the following limit is well-defined and non-zero:

$$\forall \gamma \in \mathcal{P}, \varepsilon \in \mathcal{I}^*(\gamma) : \quad \varphi_{\mathcal{P} \setminus \{\varepsilon\}}^{\gamma}(-\vec{\rho}) := \lim_{\gamma \in \Lambda \nearrow \mathcal{P} \setminus \{\varepsilon\}} \varphi_{\mathcal{P} \setminus \{\varepsilon\}}^{\gamma}(-\vec{\rho}) > 0. \quad (31)$$

Fix $\Lambda \in \mathcal{P}$. As (\mathcal{P}, \approx) is connected, there is at least one polymer $\xi_{|\Lambda|} \in \Lambda$ with $(\Lambda, \xi_{|\Lambda|})$ escaping. Iterating this argument, for $\Lambda \setminus \{\xi_{|\Lambda|}\}$, we obtain

$$\Xi_{\Lambda}(\vec{z}) = \prod_{i=1}^n \varphi_{\Lambda_i}^{\xi_i}(\vec{z}), \quad (32)$$

where $\Lambda_i := \{\xi_1, \dots, \xi_i\}$ and all factors are escaping. Therefore (31) implies $\vec{\rho} \in \mathcal{R}_{\mathcal{P}}$.

In the second part we show that $\vec{\rho} \phi_{\gamma}^{\text{red}}(\vec{\mu}) \leq \vec{\mu}$ (22) implies

$$\forall \gamma \in \mathcal{P}, \varepsilon \in \mathcal{I}^*(\gamma), \gamma \in \Lambda \Subset \mathcal{P} \setminus \{\varepsilon\} : \quad \varphi_{\Lambda}^{\gamma}(-\vec{\rho}) \geq \frac{1}{1 + \mu_{\gamma}}. \quad (33)$$

The claim follows by induction over $|\Lambda|$, simultaneously over all $\gamma \in \mathcal{P}$ and $\varepsilon \in \mathcal{I}^*(\gamma)$. The induction base is

$$\varphi_{\{\gamma\}}^{\gamma}(-\vec{\rho}) = 1 - \rho_{\gamma} \geq 1 - \frac{\mu_{\gamma}}{\phi_{\gamma}^{\text{red}}(\vec{\mu})} \geq 1 - \frac{\mu_{\gamma}}{1 + \mu_{\gamma}} = \frac{1}{1 + \mu_{\gamma}}.$$

For the induction step let (Λ, γ) be escaping and set $\{\xi_1, \dots, \xi_m\} := \Lambda \cap \mathcal{I}^*(\gamma)$. Then $m \leq D_{\gamma} - 1$ and every $(\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}, \xi_i)$ on the rhs of (29b) is escaping, too. Hence

$$\begin{aligned} & \varphi_{\Lambda}^{\gamma}(-\vec{\rho}) \\ &= 1 - \frac{\rho_{\gamma}}{\prod_{i=1}^m \varphi_{\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}}^{\xi_i}(-\vec{\rho})} && \text{by (29b)} \\ &\geq 1 - \frac{\rho_{\gamma}}{\prod_{i=1}^m (1 - \mu_{\xi_i})^{-1}} && \text{by induction} \\ &\geq 1 - \frac{\mu_{\gamma}}{1 + \mu_{\gamma}} \times \frac{\min_{\varepsilon \in \mathcal{I}^*(\gamma)} \prod_{\xi' \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}} (1 + \mu_{\xi'})^{-1}}{\prod_{i=1}^m (1 - \mu_{\xi_i})^{-1}} && \text{by (22)} \\ &\geq 1 - \frac{\mu_{\gamma}}{1 + \mu_{\gamma}} \times 1 && \text{cancelling} \\ &= \frac{1}{1 + \mu_{\gamma}}. \end{aligned}$$

□

Example 7. We show that there is a polymer system, on which the analyticity of the one polymer partition ratios breaks down in the limit at a boundary point of $\mathcal{R}_{\mathcal{P}}$, for a non-physical negative fugacity.

Let (\mathcal{P}, \approx) be isomorph to an infinite D -regular tree, modulo the loops at each vertex. Fix an end E , that is an equivalence class of rays, of the tree. For $\gamma \in \mathcal{P}$, let F_{γ} be the set of polymers further away from E than γ . These are the polymers, for which the ray starting at the polymer and being equivalent to E , passes through γ . We have the decomposition

$$F_{\gamma} := \{\gamma\} \uplus \biguplus_{\xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}} F_{\xi}, \quad (34a)$$

where ε is the unique polymer incompatible with γ which is closer to E than γ . Homogeneous fugacity $\rho \vec{1}$ and the transitivity of (\mathcal{P}, \approx) imply that

$$\alpha(\rho) := \varphi_{F_{\gamma}}^{\gamma}(-\rho \vec{1}) \quad (34b)$$

is well-defined for $\rho \leq \frac{(D-1)^{(D-1)}}{D^D} := \rho^*$ [She85]. The fundamental identity (29b) yields

$$\alpha(\rho) = 1 - \frac{\rho}{\alpha(\rho)^{D-1}}. \quad (34c)$$

By (30a) we have the limit

$$\lim_{\rho \rightarrow \rho^*} \alpha(\rho) = \alpha(\rho^*) = \frac{D-1}{D}. \quad (34d)$$

But the derivative is

$$\left(\frac{\partial \alpha}{\partial z} \right) (\rho) = \frac{1}{\alpha(\rho)^{D-2} D [\alpha(\rho^*) - \alpha(\rho)]} \quad (34e)$$

and diverges as we approach ρ^*

$$\lim_{\rho \rightarrow \rho^*} \left(\frac{\partial \alpha}{\partial z} \right) (\rho) = \infty. \quad (34f)$$

4 The tree-operator framework

This section reviews the tree-operator framework. The two key ingredients are Penrose's identity in section 4.1 and tree-operators in section 4.3. They work together in the following way: Penrose's identity rewrites each Ursell function as a finite sum over a finite family of trees. We then enlarge the family by cutting each tree into depth k pieces and only keeping constraints within those pieces. The relaxed constraints allow us to write a weighted series over Ursell functions, as appearing in a cluster expansion, as the limit of a repeated application of a depth k tree-operator. The tree-operator builds the enlarged family of weighted trees by summing over all possible reassemblings of trees from the above pieces.

The above weighted series converges iff the tree-operator has a finite fixpoint. In section 4.2 we recapitulate a classic fixpoint theorem by Tarski. A sufficient condition for the fixpoint theorem then becomes a SCUB for the polymer system. Section 4.4 exemplates this procedure by spelling out a generic depth k SCUB for the pinned series.

4.1 Penrose's identity

Let $G := (V, E)$ be a finite, simple graph. Then \mathcal{C}_G is the *poset of all spanning subgraphs* of G with *partial order* given by

$$H \leq H' \Leftrightarrow E(H) \subseteq E(H').$$

For $L, U \in \mathcal{C}_G$ with $L \leq U$, the *interval* from L to U is defined as

$$[L, U] := \{H \in \mathcal{C}_G : L \leq H \leq U\}.$$

A particular subset of \mathcal{C}_G is \mathcal{T}_G , the *set of all spanning trees* of G . A function $S : \mathcal{T}_G \rightarrow \mathcal{C}_G$ is a *partition scheme* of \mathcal{C}_G [Pen67, before (5)] iff

$$\mathcal{C}_G := \bigsqcup_{T \in \mathcal{T}_G} [\mathbb{T}, S(T)]. \quad (35)$$

Define the *set of singleton trees with respect to S* (short *S -trees*) by

$$\mathcal{T}_S(G) := \{\mathbb{T} \in \mathcal{T}_G : \mathbb{T} = S(\mathbb{T})\}. \quad (36)$$

Theorem 8 (Penrose [Pen67, equation (5)]). *If S is a partition scheme of \mathcal{C}_G , then*

$$\sum_{H \in \mathcal{C}_G} (-1)^{|E(H)|} = (-1)^{|V|-1} |\mathcal{T}_S(G)|. \quad (37)$$

The number of S -trees is independent of the choice of S .

Proof. Let $(x_e)_{e \in E}$ be a vector of numbers. Then

$$\begin{aligned} \sum_{H \in \mathcal{C}_G} \prod_{e \in E(H)} x_e &= \sum_{\mathbb{T} \in \mathcal{T}_G} \prod_{e \in E(\mathbb{T})} x_e \sum_{F \subseteq E(S(\mathbb{T})) \setminus E(\mathbb{T})} \prod_{f \in F} x_f \\ &= \sum_{\mathbb{T} \in \mathcal{T}_G} \prod_{e \in E(\mathbb{T})} x_e \prod_{f \in E(S(\mathbb{T})) \setminus E(\mathbb{T})} (1 + x_f). \end{aligned}$$

Set all $x_e = -1$. This cancels all the contributions from trees with $\mathbb{T} \neq S(\mathbb{T})$, while for every $\mathbb{T} \in \mathcal{T}_S(G)$ the contribution is $(-1)^{|V|-1}$. \square

4.2 A fixpoint theorem

In this section we present an adaption of a well known fixpoint theorem on lattices by Tarski [Tar55]. For some countable set of labels \mathcal{L} , let $X := [0, \infty]^\mathcal{L}$ be the *lattice* with *partial order* $\vec{x} \leq \vec{y}$, that is coordinate-wise comparison of the vectors: $\forall l \in \mathcal{L} : x_l \leq y_l$.

We say that a function $\phi : X \rightarrow X$ *preserves the order* iff

$$\forall \vec{x}, \vec{y} \in X : \quad \vec{x} \leq \vec{y} \Rightarrow \phi(\vec{x}) \leq \phi(\vec{y}). \quad (38)$$

The set of *decreasing points* of ϕ is

$$D_\phi := \{\vec{y} \in X : \phi(\vec{y}) \leq \vec{y}\}. \quad (39)$$

A sequence $(\vec{y}^{(n)})_{n \in \mathbb{N}}$ of elements of X is said to be *non-decreasing* and *non-increasing* iff $\forall n \in \mathbb{N} : \vec{y}^{(n)} \leq \vec{y}^{(n+1)}$ and $\vec{y}^{(n)} \geq \vec{y}^{(n+1)}$ respectively.

Proposition 9 (after [FP07, proposition 8]). *Let $\phi : X \rightarrow X$ be order-preserving. If there is a $\vec{\mu} \in D_\phi$, then $(\phi^n(\vec{0}))_{n \in \mathbb{N}_0}$ is non-decreasing with limit $\vec{\rho}^*$, $(\phi^n(\vec{\mu}))_{n \in \mathbb{N}_0}$ is non-increasing with limit $\vec{\mu}^*$ and we have*

$$\phi(\vec{\rho}^*) = \vec{\rho}^* \leq \vec{\mu}^* = \phi(\vec{\mu}^*). \quad (40)$$

In particular, $\vec{\rho}^ \in [0, \infty]^\mathcal{L}$ iff $D_\phi \cap [0, \infty]^\mathcal{L} \neq \emptyset$.*

4.3 Depth k tree-operators

The aim of this section is to show a generic result for depth k recursive constructions of weighted, labelled, finite trees and convergence of certain series of those trees. It generalizes [FP07, proposition 8 and parts of proposition 7].

Let $\mathfrak{T}_n^=$ be the set of rooted, finite trees of depth n , $\mathfrak{T}_n^{\leq} := \biguplus_{m \leq n} \mathfrak{T}_m^=$ the set of rooted, finite trees of depth at most n and $\mathfrak{T}_{\infty}^{\leq} := \biguplus_{m \in \mathbb{N}_0} \mathfrak{T}_m^=$ the set of rooted, finite trees. Denote by $\mathfrak{p}(t)$ the number of rooted automorphisms of t (they fix the root). Let \mathcal{L} be a countable set of labels. A function $c : \mathcal{L}^{V(t)} \rightarrow [0, \infty[$ is t -invariant iff it is invariant under all rooted automorphism of t . We denote by $L_i(t)$ the i -th level of t and by $W(t)$ the non-root vertices of t . Finally t_k^v is the rooted subtree of t with root v and depth k .

Let \mathcal{T}_n be the set of trees with vertex set $[n]_0$ and root 0. Consequently $\mathcal{T}_{\infty} := \biguplus_{n \geq 0} \mathcal{T}_n$. For $\tau \in \mathcal{T}_{\infty}$ we denote its unlabelled version by $t(\tau) \in \mathfrak{T}_{\infty}^{\leq}$.

Proposition 10. Fix $k \in \mathbb{N}$. Let $(c_t)_{t \in \mathfrak{T}_k^{\leq}}$ be a collection of non-negative functions, with each c_t being t -invariant. Let $X := [0, \infty]^{\mathcal{L}}$ and $\vec{\rho} \in X$. Consider the operator $T_{\vec{\rho}} : X \rightarrow X$, defined $\forall l \in \mathcal{L}$ by

$$\vec{\mu} \mapsto [T_{\vec{\rho}}(\vec{\mu})]_l := \sum_{t \in \mathfrak{T}_k^{\leq}} \frac{1}{\mathfrak{p}(t)} \sum_{\vec{\lambda} \in \{l\} \times \mathcal{L}^{|W(t)|}} c_t(\vec{\lambda}) \prod_{\substack{v \in L_i(t) \\ 0 \leq i \leq k-1}} \rho_{\lambda_v} \prod_{w \in L_k(t)} \mu_{\lambda_w}. \quad (41a)$$

If there exists $\vec{\mu} \in X$ such that

$$T_{\vec{\rho}}(\vec{\mu}) \leq \vec{\mu}, \quad (41b)$$

then the family of series, indexed by \mathcal{L} ,

$$R_l(\vec{\rho}) := \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\lambda} \in \{l\} \times \mathcal{L}^n} \sum_{\tau \in \mathcal{T}_n} \prod_{\substack{i \in [n]_0 \\ d_{\tau}(0, i) = 0 \bmod k}} c_{t(\tau_k^i)}(\vec{\lambda}_{V(\tau_k^i)}) \prod_{j=0}^n \rho_{\lambda_j} \quad (41c)$$

converges uniformly, as

$$R(\vec{\rho}) = \lim_{n \rightarrow \infty} T_{\vec{\rho}}^n(\vec{\rho}) = T_{\vec{\rho}}(R(\vec{\rho})) \leq \vec{\mu}. \quad (41d)$$

Proof. Omitting some tedious rewriting of $R(\vec{\rho})$, which can be found in [Tem12, section 5.4.5], we obtain that $\forall l \in \mathcal{L}$:

$$[T_{\vec{\rho}}^n(\vec{0})]_l = \sum_{t \in \mathfrak{T}_{n-1}^{\leq}} \sum_{\vec{\lambda} \in \{l\} \times \mathcal{L}^{W(t)}} \sum_{m=0}^{n-1} \sum_{v \in L_{mk}(t)} \frac{c_{t_k^v}(\vec{\lambda}_{W(t_k^v)})}{\mathfrak{p}(t_k^v)} \prod_{v \in V(t)} \rho_{\lambda_v}.$$

Taking the monotone increasing limit, we see that

$$R(\vec{\rho}) = \lim_{n \rightarrow \infty} [T_{\vec{\rho}}^n(\vec{0})].$$

The operator $T_{\vec{\rho}}$ has only non-negative coefficients, hence is order preserving. Apply proposition 9 together with condition (41b) to see that $R(\vec{\rho})$ is the least fixpoint of $T_{\vec{\rho}}$ and that (41d) holds. \square

The following proposition is an extension of arguments in [BFPS11, appendix]:

Proposition 11. *Suppose that $T_{\vec{\rho}} \geq \vec{\rho}(\vec{1} + \vec{\mu})$ and (41b) holds. Decompose $T_{\vec{\rho}} =: \vec{\rho}(\text{id}_X + S_{\vec{\rho}})$ by splitting off the root of each tree. Likewise decompose $R(\vec{\rho}) =: \vec{\rho}Q(\vec{\rho})$. Then $S_{\vec{\rho}} \geq \vec{0}$ is order-preserving, $\vec{\rho} < \vec{1}$ and we refine (41d) to*

$$\forall l \in \mathcal{L} : \quad [Q(\vec{\rho})]_l \leq \frac{[S_{\vec{\rho}}(\vec{\mu})]_l}{1 - \rho_l} < \infty. \quad (42)$$

Proof. As $R(\vec{\rho})$ and $Q(\vec{\rho})$ increase in $\vec{\rho}$, we assume without loss of generality that $\vec{\mu} \geq \vec{\rho} > \vec{0}$ or fall back on a smaller polymer system omitting the 0 entries of $\vec{\rho}$. We have

$$\vec{\rho}(\vec{1} + \vec{\mu}) \leq T_{\vec{\rho}}(\vec{\mu}) \leq \vec{\mu},$$

whereby

$$\forall l \in \mathcal{L} : \quad \rho_l \leq \frac{\mu_l}{1 + \mu_l} < 1.$$

Thus

$$\vec{\rho}Q(\vec{\rho}) = R(\vec{\rho}) = T_{\vec{\rho}}(R(\vec{\rho})) = \vec{\rho}(\text{id}_X + S_{\vec{\rho}})(R(\vec{\rho})) = \vec{\rho}R(\vec{\rho}) + S_{\vec{\rho}}(R(\vec{\rho})),$$

whence, ignoring 0 entries of $\vec{\rho}$ and as $S_{\vec{\rho}}$ is order-preserving,

$$Q(\vec{\rho}) = \vec{\rho}Q(\vec{\rho}) + S_{\vec{\rho}}(R(\vec{\rho})) \leq \vec{\rho}Q(\vec{\rho}) + S_{\vec{\rho}}(\vec{\mu}).$$

□

4.4 Pinned series depth k approximation

The classic case aims to uniformly bound the so-called *pinned series*

$$\rho_\gamma \Psi_\gamma(\vec{\rho}) := \rho_\gamma \lim_{\Lambda \nearrow \mathcal{P}} \frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(-\vec{\rho}) = \rho_\gamma \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in \mathcal{P}^n} |\mathbf{u}(\gamma, \vec{\xi})| \prod_{i=1}^n (-\rho_{\xi_i}). \quad (43)$$

This section extends [FP07, proposition 7] to level k approximations. By (68) an upper bound on the pinned series is equivalent to a lower bound on the one polymer partition ratios. For basic notation see section 4.3.

Proposition 12. *Fix $k \in \mathbb{N}$. Suppose that we have a family of t -invariant functions $(c_t)_{t \in \mathfrak{T}_k^\leq}$ such that*

$$\forall \vec{\xi} \in \mathcal{P}^{n+1} : \quad |\mathbf{u}(\xi_0, \dots, \xi_n)| \leq \sum_{\tau \in \mathcal{T}_n} \prod_{\substack{i \in [n]_0 \\ d_\tau(0, i) = 0 \bmod k}} c_{t(\tau_k^i)}(\vec{\xi}_{V(\tau_k^i)}). \quad (44a)$$

Let $X := [0, \infty]^\mathcal{P}$ and $\vec{\rho} \in X$. Consider the operator $T_{\vec{\rho}} : X \rightarrow X$ defined $\forall \gamma \in \mathcal{P}$ by

$$\vec{\mu} \mapsto [T_{\vec{\rho}}(\vec{\mu})]_\gamma := \sum_{t \in \mathfrak{T}_k^\leq} \frac{1}{\mathbf{p}(t)} \sum_{\vec{\xi} \in \{\gamma\} \times \mathcal{P}^{|W(t)|}} c_t(\vec{\xi}) \prod_{\substack{v \in L_i(t) \\ 0 \leq i \leq k-1}} \rho_{\xi_v} \prod_{w \in L_k(t)} \mu_{\xi_w}. \quad (44b)$$

If there exists $\vec{\mu} \in X$ such that

$$T_{\vec{\rho}}(\vec{\mu}) \leq \vec{\mu}, \quad (44c)$$

then $\vec{\rho} < \vec{1}$ and

$$\vec{\rho}\Psi(\vec{\rho}) \leq \vec{\mu}. \quad (44d)$$

This implies that $\vec{\rho} \in \text{Int } \mathcal{R}_{\mathcal{P}}$ and $\vec{\rho} < \vec{1}$.

Proof. Setting $\mathcal{L} := \mathcal{P}$ in (41c), condition (44a) implies that

$$\begin{aligned} [\vec{\rho}\Psi(\vec{\rho})]_{\gamma} &= \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in \{\gamma\} \times \mathcal{P}^n} |\mathbf{u}(\vec{\xi})| \prod_{i=0}^n \rho_{\xi_i} \\ &\leq \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in \{\gamma\} \times \mathcal{P}^n} \sum_{\tau \in \mathcal{T}_n} \prod_{\substack{i \in [n]_0 \\ d_{\tau}(0,i) \equiv 0 \pmod{k}}} c_{t(\tau_k^i)}(\vec{\xi}_{V(\tau_k^i)}) \prod_{j=0}^n \rho_{\xi_j} = [R(\vec{\rho})]_{\gamma}. \end{aligned}$$

Then (44d) follows from (41d). The relation (69) implies that $\vec{\rho} \in \text{Int } \mathcal{R}_{\mathcal{P}}$. Finally, if $\rho_{\gamma} \geq 1$, then (30a) and the fundamental identity (29b) imply that $\varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) \leq 0$, a contradiction to $\vec{\rho} \in \text{Int } \mathcal{R}_{\mathcal{P}}$. \square

5 Explorative partition schemes

Section 4.4 shows how to majorate the pinned series with the help of a tree-operator. The tree-operator constructs the enlarged family of trees locally. For the tree-operator approximation to be tighter, it has to keep as many restrictions as possible from the original family of singleton trees. This is easier, if the partition scheme places primarily local restrictions on its singleton trees. This section describes such schemes.

We recall some facts about the anatomy of a cluster in section 5.1. The motivation and description of explorative partition schemes, which have the above outlined qualities, are in section 5.2. They built upon the implicit breadth-first search algorithm present in Penrose's partition scheme, which we recast in the explorative style in section 5.3. Our new partition scheme, which advances selectively based on the structure of the cluster, is in section 5.4. Finally, we outline the main parts of an explorative partition scheme interpolating between the greedy behaviour of Penrose's partition scheme and our new partition scheme in section 5.5.

5.1 The anatomy of a cluster

Let I be a finite set and $G(\vec{\xi})$ be the *induced graph* of $\vec{\xi} \in \mathcal{P}^I$. We emphasise the fact, that the coarse structure of $G(\vec{\xi})$ resembles the one of the polymer subsystem $(\text{supp } \vec{\xi}, \approx)$ of its support. See figure 5 for an example. Formally, there is a polymer partition $(C_{\gamma})_{\gamma \in \text{supp } \vec{\xi}}$ of I , with

$$\forall \gamma \in \text{supp } \vec{\xi}: \quad C_{\gamma} := \{i \in I : \xi_i = \gamma\}. \quad (45)$$

The graph $G(C_{\gamma})$ is a complete subgraph of $G(\vec{\xi})$. For two distinct polymers $\gamma, \gamma' \in \text{supp } \vec{\xi}$ there are either no edges at all between C_{γ} and $C_{\gamma'}$, that is $E(C_{\gamma}, C_{\gamma'}) = \emptyset$ iff $\gamma \not\approx \gamma'$, or all possible edges are present, that is iff $\gamma \approx \gamma'$. It follows that $G(\vec{\xi})$ is connected iff $(\text{supp } \vec{\xi}, \approx)$ is, and in this case $G(\vec{\xi})$ is a *cluster*.

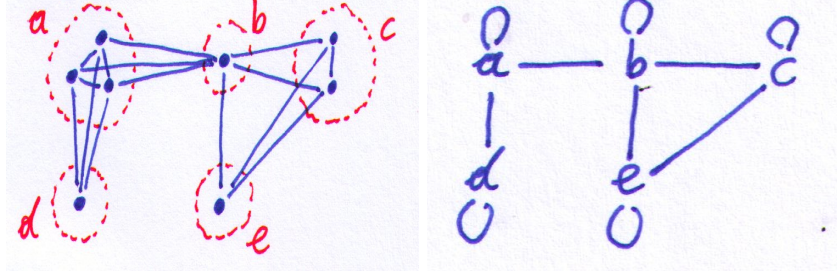


Figure 5: Anatomy of the cluster of $G((a, a, b, c, a, d, c, e))$ on the left, for the incompatibility graph of its support $(\{a, b, c, d, e\}, \approx)$ on the right. We clearly distinguish the structural constraints $G((a, a, b, c, a, d, c, e))$ inherits from $(\{a, b, c, d, e\}, \approx)$.

5.2 The basic idea

Let $G := (V, E)$ be a simple graph. The aim of this section is to introduce partition schemes of \mathcal{C}_G described by an exploration algorithm. The algorithm selects a spanning tree from a spanning subgraph. It does so by an iterative exploration of the subgraph. The complement to the algorithm is a sufficient compatibility condition to uniquely reconstruct the maximal subgraph reducing to a given spanning tree from said spanning tree.

Given $H \in \mathcal{C}_G$ and a root o , the generic *exploration algorithm* \mathcal{E}_{Gen} [13](#) selects a spanning tree of H by starting at a root o and growing the tree iteratively: during each iteration it considers all the nodes neighbouring its deepest level, selects at least one of those neighbours, adds each selected vertex and one of the edges leading to it to the tree and removes all superfluous edges, including those to ignored vertices. This prescription guarantees the selection of a spanning tree of H (see [proposition 15](#)).

We discriminate between two types of information: the *static information* is our knowledge of the structure of G , the choice of the root o and all other information we may have about G , like labellings or orderings of elements. The *dynamic information* is the information we gather about H during its exploration, including properties as connectedness and selection of vertices.

The complementary procedure takes a tree $\mathbb{T} \in \mathcal{T}_G$ and partitions $E \setminus E(\mathbb{T})$ into the *admissible edges* $\mathcal{A}_{Gen}(\mathbb{T})$ and the *conflicting edges* $\mathcal{C}_{Gen}(\mathbb{T})$. If this partition is compatible [\(47\)](#) with the exploration algorithm [13](#), then the preimage of the \mathcal{E}_{Gen} defines a partition scheme Gen (see [proposition 16](#)). The compatibility is satisfied iff all the dynamic information used in \mathcal{E}_{Gen} to select at vertex on level n of the \mathbb{T} from H is a function of the first n levels of \mathbb{T} (and the static information).

A partition scheme is *explorative* iff it can be described in the above way. The motivation for the formalisation of explorative partition schemes is that the exploration algorithm [13](#) advances locally through the graph. Hence we hope

to deduce local properties of the singleton trees of such a scheme from the local structural properties of G .

In the rest of this section we formalise and prove the correctness of the outlined idea, resulting in the generic explorative partition scheme *Gen*. We fill the gaps in *Gen*'s specification in later sections, resulting in different partition schemes.

Algorithm 13 (*Gen* exploration). Let $H \in \mathcal{C}_G$. We construct a sequence $(H_k)_{k \in \mathbb{N}_0}$ of subgraphs of H starting with $H_0 := H$ and a sequence $(T_k)_{k \in \mathbb{N}_0}$ of subsets of V starting with $T_0 := \{o\}$. We think of T_k as the *explored tree* part of H_k . We construct H_{k+1} from H_k by the following steps:

- (gb) Let the *unexplored part* be $U_k := V \setminus T_k$. Let the *potential nodes* P_k be the set of neighbours of T_k in U_k and the *boundary* B_k be the set of neighbours of U_k in T_k . SELECT a subset S_k of P_k , containing at least one vertex from $C \cap P_k$ for every connected component C of $H_k|_{U_k}$. Call these the *selected nodes*. Set $T_{k+1} := T_k \uplus S_k$.
- (gi) Let the *ignored nodes* be $I_k := P_k \setminus S_k$. REMOVE all the edges in $E(B_k, I_k) \cap E(H_k)$.
- (gp) For each $v \in S_k$ SELECT $(v, w_v) \in E(B_k, S_k) \cap E(H_k)$.
- (gu) For each $v \in S_k$ REMOVE all $(v, w_v) \neq (v, w) \in E(B_k, S_k) \cap E(H_k)$.
- (gc) REMOVE all of $E(S_k) \cap E(H_k)$.

See also figure 6.

Remark. Observe that all steps factorise over connected components of $H_k|_{U_k}$. We can schedule the iterations on different connected components in parallel and in arbitrary order. We can advance further into one connected component and explore it further without independently of the exploration of the other connected components.

Proposition 14. *The following invariants hold $\forall k \in \mathbb{N}_0$ in algorithm 13:*

$$H_{k+1} \leq H_k \tag{46a}$$

$$H_k|_{T_k} \text{ is a tree} \tag{46b}$$

$$H_k \in \mathcal{C}_G \tag{46c}$$

$$H_{k+1}|_{T_k} = H_k|_{T_k} \tag{46d}$$

$$H_k|_{U_k} = H|_{U_k} \tag{46e}$$

$$(E(U_k) \uplus E(U_k, B_k)) \cap E(H_k) = (E(U_k) \uplus E(U_k, B_k)) \cap E(H) \tag{46f}$$

$$\forall l \geq k : \quad v \in S_k \Leftrightarrow d_{H_l}(o, v) = k \tag{46g}$$

$$B_{k+1} \subseteq S_k \tag{46h}$$

Remark. We can replace every occurrence of $E(H_k)$ by $E(H)$ in algorithm 13. This follows from invariant (46f), which asserts that for each edge there is exactly one iteration of the exploration algorithm during which it is either selected or removed.

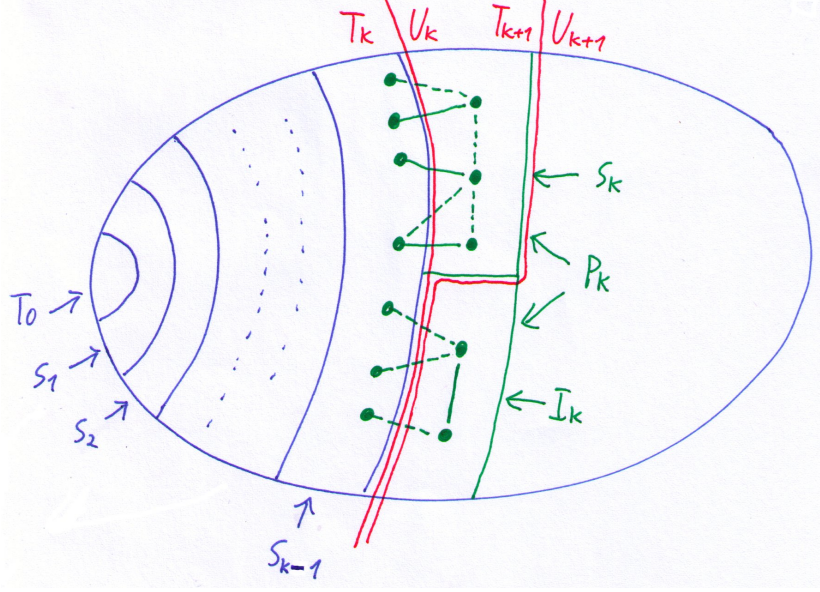


Figure 6: The generic exploration algorithm 13 constructing H_{k+1} from H_k . The notation is from algorithm 13.

Proof. Invariant (46a) is clear as we obtain H_{k+1} from H_k by removing edges. Invariant (46e) follows from (46f). Invariant (46d) follows from (46b) and the subgraph relationship (46a).

(46h): (gi) ensures that all connections in H_{k+1} between B_k and U_{k+1} go over S_k . By induction these are all connections in H_{k+1} between T_k and U_{k+1} .

We prove the other invariants by induction. They all hold trivially for $k = 0$.

(46b): The subgraph $H_{k+1}|_{T_{k+1}}$ consists of $H_{k+1}|_{T_k}$, the vertices S_k and the edge sets $E(T_k, S_k) \cap E(H_{k+1})$ and $E(S_k) \cap E(H_{k+1})$. By (46d) and (46b) $H_{k+1}|_{T_k} = H_k|_{T_k}$ is a tree. (gc) ensures that $E(S_k) \cap E(H_{k+1}) = \emptyset$. (gp) and (gu) ensure that each $v \in S_k$ has a unique neighbour in T_k in $H_{k+1}|_{T_{k+1}}$. Thus $H_{k+1}|_{T_{k+1}}$ is a tree.

(46c): The tree $H_{k+1}|_{T_{k+1}}$ (46b) is connected. If $v \in U_{k+1}$, then (gb) asserts that there exists a connected component C of $H_k|_{U_k}$ such that $v \in C$. (gb) also asserts that there exists a $w \in C \cap S_k$ such that: (gp) asserts that there exists a $z \in T_k$ with $z \sim w$ in H_k and from (46e) it follows that $H_{k+1}|_{U_{k+1}} = H_k|_{U_{k+1}}$. Thus $v \leftrightarrow w \leftrightarrow z \leftrightarrow o$ and H_{k+1} is connected.

(46f): During iteration k (gi), (gu) and (gc) only remove edges in $E(B_k, P_k)$ or $E(S_k)$. Thus $E(U_{k+1}) \cap E(H_k)$ and by (46g) $E(B_{k+1}, U_{k+1}) \cap E(H_k) = E(S_k, U_{k+1}) \cap E(H_k)$ are subsets of $E(H_{k+1})$. The statement (46f) follows by induction over k .

(46g): If $v \in T_k$, then $d_{H_{k+1}}(o, v) = d_{H_k}(o, v) = k$, as $H_{k+1}|_{T_k} = H_k|_{T_k}$ by (46d). It rests to show that

$$v \in S_k \Leftrightarrow d_{H_{k+1}}(o, v) = k + 1.$$

If $d_{H_{k+1}}(o, v) = k + 1$, then $v \notin T_k := \biguplus_{l=0}^k B_k$ and there exists a w with $(v, w) \in E(H_{k+1})$ and $d_{H_{k+1}}(o, w) = k$. Thus $w \in B_k$. By (gi) and (gu) the only neighbours of B_k in U_k in the graph H_{k+1} are those in S_k .

On the other hand if $v \in S_k$, then, as $H_{k+1}|_{T_{k+1}}$ is a tree (46b), it has a unique parent $w \in B_k \subseteq S_{k-1}$ (46h). As w is v 's only neighbour at distance k from the root in H_{k+1} (46g) we have $d_{H_{k+1}}(o, v) = d_{H_{k+1}}(o, w) + 1 = k + 1$. \square

Proposition 15. *Algorithm 13 describes a function $\mathcal{E}_{Gen} : \mathcal{C}_G \rightarrow \mathcal{T}_G$. It is monotone decreasing, that is $\forall H \in \mathcal{C}_G : \mathcal{E}_{Gen}(H) \leq H$.*

Proof. Let $H \in \mathcal{C}_G$ and apply algorithm 13 to it. We observe that if $T_k = V$, then $H_k = H_{k+1}$. But as long as $T_k \neq V$ we have $S_k \neq \emptyset$ (as $H_k \in \mathcal{C}_G$ by (46a)) and therefore $(T_k)_{k \in \mathbb{N}_0}$ grows strictly monotone to and then stabilises in V in at most $|V|$ steps. This implies that the monotone decreasing (46a) sequence $(H_k)_{k \in \mathbb{N}_0}$ of subgraphs of H stabilises in $H_{|V|}$. Finally (46b) asserts that $H_{|V|} = H_{|V|}|_{T_{|V|}}$ is a tree and (46c) that $H_{|V|} \in \mathcal{C}_H$ and thus $H_{|V|} \leq H$. \square

Proposition 16. *Let \mathcal{E}_{Gen} be as in proposition 15. For each $\mathbb{T} \in \mathcal{T}_G$, partition $E(\mathbb{T})$ into the admissible edges $\mathcal{A}_{Gen}(\mathbb{T})$ and the conflicting edges $\mathcal{C}_{Gen}(\mathbb{T})$. If, for each $H \in \mathcal{E}_{Gen}^{-1}(\mathbb{T})$, we have*

$$\forall e \in \mathcal{A}_{Gen}(\mathbb{T}) \setminus E(H) : \quad \mathcal{E}_{Gen}((V, E(H) \uplus \{e\})) = \mathbb{T} \quad (47a)$$

and

$$\forall C \subseteq \mathcal{C}_{Gen}(\mathbb{T}) \setminus E(H) : \quad \mathcal{E}_{Gen}((V, E(H) \uplus C)) \neq \mathbb{T}, \quad (47b)$$

then the map

$$Gen : \mathcal{T}_G \rightarrow \mathcal{C}_G \quad \mathbb{T} \mapsto Gen(\mathbb{T}) := (V, E(\mathbb{T}) \uplus \mathcal{A}_{Gen}(\mathbb{T})) \quad (48)$$

is a partition scheme of G with $[\mathbb{T}, Gen(\mathbb{T})] = \mathcal{E}_{Gen}^{-1}(\mathbb{T})$.

Proof. Fix $\mathbb{T} \in \mathcal{T}_G$. For $A \subseteq \mathcal{A}_{Ret}(\mathbb{T})$ and $C \subseteq \mathcal{C}_{Ret}(\mathbb{T})$ let $H_{(A,C)} := (V, E(\mathbb{T}) \uplus A \uplus C)$. We show that $H_{(A,C)} \in [\mathbb{T}, Gen(\mathbb{T})]$ iff $C = \emptyset$.

First, assume that $C = \emptyset$. We argue by induction over the cardinality of A . For the induction base with $A = \emptyset$ we have $H_{(\emptyset, \emptyset)} = \mathbb{T}$ and $\mathcal{E}_{Gen}(\mathbb{T}) = \mathbb{T}$. For the induction step consider $A := A' \uplus \{e\}$. By the induction hypothesis $\mathcal{E}_{Gen}(H_{(A', \emptyset)}) = \mathbb{T}$. As $e \in \mathcal{A}_{Gen}(\mathbb{T})$ we apply (47a) to see that $\mathcal{E}_{Gen}(H_{(A, \emptyset)}) = \mathbb{T}$, too.

Secondly, assume that $C \neq \emptyset$. We already showed that $\mathcal{E}_{Gen}(H_{(A, \emptyset)}) = \mathbb{T}$. Therefore (47b) implies that $\mathcal{E}_{\mathbb{T}}(H_{(A,C)}) \neq \mathbb{T}$. \square

5.3 The Penrose or greedy scheme

Let I be a finite and totally ordered set. Let $G := (I, E)$ be a connected graph. We present a formulation of the first partition scheme by Penrose [Pen67, equation (6)] or [FP07, section 4.1] in the explorative style of section 5.2. The static information comprises the total order on I , the structure of G and the choice of the root $o \in I$.

We call *Pen* also *greedy* because of the choice of S_k in (pb). Algorithm 17 flood-fills H . This means it incorporates a parallel version of *Dijkstra's single-source shortest path algorithm* [Dij59], [KV06, page 145] on a graph with unit edge weights.

Algorithm 17 (*Pen* exploration). Let $H \in \mathcal{C}_G$. For every k , let H_k, T_k, U_k, B_k and P_k be as in algorithm 13. The missing specification to go from H_k to H_{k+1} on a connected component C of $H_k|_{U_k}$ is:

(pb) SELECT $C \cap S_k := C \cap P_k$.

(pi) As $C \cap I_k = \emptyset$ REMOVE nothing.

(pp) For $i \in C \cap S_k$ let $j_i := \operatorname{argmin} \{j \in B_k : (i, j) \in E(H_k)\}$. SELECT (i, j_i) .

(pu) For $i \in C \cap S_k$ REMOVE all $(i, j) \in E(H_k)$ with $j_i \neq j \in B_k$.

(pc) REMOVE all of $E(C \cap S_k) \cap E(H_k)$.

Proposition 18. *The function \mathcal{E}_{Pen} described in algorithm 17 is $\mathcal{C}_G \rightarrow \mathcal{T}_G$ and monotone decreasing, that is $\forall H \in \mathcal{C}_G : \mathcal{E}_{Pen}(H) \leq H$.*

Proof. Follows from proposition 15. □

Algorithm 19 (*Pen* tree edge complement partition). Let $\mathbb{T} \in \mathcal{T}_G$. Let L_k be the k^{th} level of \mathbb{T} . We partition $E \setminus E(\mathbb{T})$ into $\mathcal{A}_{Pen}(\mathbb{T}) \uplus \mathcal{C}_{Pen}(\mathbb{T})$. Let $0 \leq k \leq l, j \in L_k, i \in L_l$ and $e := (i, j) \in E \setminus E(\mathbb{T})$. Then $e \in \mathcal{C}_{Pen}(\mathbb{T})$ iff one of the mutually exclusive conditions (49) holds:

$$l \geq k + 2, \tag{49a}$$

$$l = k + 1 \wedge j < \mathbf{p}(i). \tag{49b}$$

And $e \in \mathcal{A}_{Pen}(\mathbb{T})$ iff one of the mutually exclusive conditions (50) holds:

$$k = l, \tag{50a}$$

$$l = k + 1 \wedge j > \mathbf{p}(i). \tag{50b}$$

Proposition 20. *The map*

$$Pen : \mathcal{T}_G \rightarrow \mathcal{C}_G \quad \mathbb{T} \mapsto Pen(\mathbb{T}) := (I, E(\mathbb{T}) \uplus \mathcal{A}_{Pen}(\mathbb{T})) \tag{51}$$

is a partition scheme of G with $[\mathbb{T}, Pen(\mathbb{T})] = \mathcal{E}_{Pen}^{-1}(\mathbb{T})$.

The proof of proposition 20 is in appendix 9. We specialize to the case of $G := G(\vec{\xi})$ being the cluster induced by a vector $\vec{\xi} \in \mathcal{P}^I$. This increases the static information about G – its structure is a function of $\vec{\xi}$.

Proposition 21 (Properties of $\mathcal{T}_{Pen}(G(\vec{\xi}))$). *Let $\mathbb{T} \in \mathcal{T}_{Pen}(G(\vec{\xi}))$ and let C_i be the set of children of i in \mathbb{T} . Then*

$$\forall k \in \mathbb{N}_0 : \quad \text{supp } \vec{\xi}_{L_k} \text{ is an independent subset of } \mathcal{P} \quad (52a)$$

$$\text{supp } \vec{\xi}_{C_i} \text{ is an independent subset of } \mathcal{I}(\xi_i) \quad (52b)$$

$$|C_i| = |\text{supp } \vec{\xi}_{C_i}|. \quad (52c)$$

Proof. Fix k . Suppose we have $i, j \in L_k$ with $\xi_i \approx \xi_j$, then $e := (i, j) \in E$ as $G = G(\vec{\xi})$ is the cluster of $\vec{\xi}$. Hence by (50a) $e \in E(Pen\mathbb{T})$ and thus $Pen(\mathbb{T}) \neq \mathbb{T}$. This shows (52a), which implies (52b), which in turn implies (52c). \square

5.4 The returning scheme

Let I be a finite and totally ordered set. Let $\vec{\xi} \in \mathcal{P}^I$ and $G := G(\vec{\xi})$. Assume that G is connected, that is it is a cluster. We present an explorative partition scheme *Ret* adapted to clusters. The static information comprises the total order on I , the cluster structure of G given by $\vec{\xi}$ and the choice of the root $o \in I$.

The partition scheme is called *returning*, because it prefers to select children with a different polymer label. This preference creates loops back to the same C_γ partition of H , if possible. For the singleton trees, this means that polymer labels of paths from the root do *not return* to the same label (after having left it). In particular we do not return to the last visited different label, which gives us a similar effect as the *escaping pairs* in the section 3. The key idea of this section is the conceptual duality between: the explorative algorithm should do – what I do not want to have in the singleton trees. See proposition 26 for the exact properties of the singleton trees.

Algorithm 22 (*Ret* exploration). Let $H \in \mathcal{C}_G$. For every k , let H_k, T_k, U_k, B_k and P_k be as in algorithm 13. The missing parts to construct H_{k+1} from H_k are:

Call an edge $(i, j) \in E(C \cap P_k, B_k) \cap E(H)$ *same* (or **S**) iff $\xi_i = \xi_j$ and *different* (or **D**) iff $\xi_i \neq \xi_j$. Likewise call a vertex $i \in P_k$ *same* iff all such (i, j) are *same* and *different* iff there exists such a non-*same* (i, j) . Finally we say that a connected component C of $H_k|_{U_k}$ is *same* iff all vertices in $C \cap P_k$ are *same* and *different* iff $C \cap P_k$ contains at least one *different* vertex.

If C is an **S** connected component of $H_k|_{U_k}$:

(**rbs**) SELECT $C \cap S_k := C \cap P_k$.

(**ris**) As $C \cap I_k = \emptyset$ REMOVE nothing.

(**rps**) For $i \in C \cap S_k$ let $j_i := \text{argmin} \{j \in B_k : (i, j) \in E(H_k)\}$. SELECT (i, j_i) .

(**rus**) For $i \in C \cap S_k$ REMOVE all $(i, j) \in E(H_k)$ with $j_i \neq j \in B_k$.

(**rbs**) REMOVE all of $E(C \cap S_k) \cap E(H_k)$.

If C is a **D** connected component of $H_k|_{U_k}$:

(**rbd**) SELECT $C \cap S_k := \{i \in C \cap P_k : i \text{ is } \mathbf{D}\}$.

- (rid) $C \cap I_k = \{i \in C \cap P_k : i \text{ is } \mathbf{S}\}$. REMOVE all of $E(B_k, (C \cap I_k)) \cap E(H_k)$.
- (rpd) For $i \in C \cap S_k$ let $j_i := \operatorname{argmin} \{j \in B_k : (i, j) \in E(H_k) \text{ is } \mathbf{D}\}$. SELECT (i, j_i) .
- (rudd) For $i \in C \cap S_k$ REMOVE every $\mathbf{D} (i, j) \in E(H_k)$ with $j_i \neq j \in B_k$.
- (ruds) For $i \in C \cap S_k$ REMOVE every $\mathbf{S} (i, j) \in E(C \cap S_k, B_k) \cap E(H_k)$.
- (rcd) REMOVE all of $E(C \cap S_k) \cap E(H_k)$.

Proposition 23. *The function \mathcal{E}_{Ret} described in algorithm 22 is $\mathcal{C}_G \rightarrow \mathcal{T}_G$ and $\mathcal{E}_{Ret}|_{\mathcal{T}_G} = id_{\mathcal{T}_G}$.*

Proof. Follows from proposition 15. □

Algorithm 24 (*Ret tree edge complement partition*). Let $\mathbb{T} \in \mathcal{T}_G$. Let L_k be the k^{th} level of \mathbb{T} . First we determine if an edge $(\mathbf{p}(i), i)$ is a same or non-same edge:

$$s : I \setminus \{o\} \rightarrow \{\mathbf{S}, \mathbf{D}\} \quad i \mapsto \begin{cases} \mathbf{S} & \xi_i = \xi_{\mathbf{p}(i)} \\ \mathbf{D} & \xi_i \neq \xi_{\mathbf{p}(i)} \end{cases} \quad (53)$$

For $k \geq 1$ define the *equivalence relation* $\sim_{(k)}$ on L_k by

$$i \sim_{(k)} j \Leftrightarrow s(P(o, i) \setminus \{o\}) = s(P(o, j) \setminus \{o\}), \quad (54)$$

where the equality on the rhs is taken in $\{\mathbf{S}, \mathbf{D}\}^k$. This implies that an equivalence class consists of either only same or only non-same nodes and whence we can extend s to them. For completeness let $\sim_{(0)}$ be the trivial equivalence relation on $L_0 = \{o\}$. The equivalence classes possess a *tree structure* consistent with \mathbb{T} :

$$i \sim_{(k+1)} j \Rightarrow \mathbf{p}(i) \sim_{(k)} \mathbf{p}(j), \quad (55)$$

that is equivalent vertices in L_{k+1} have equivalent parents in L_k . We therefore call $[\mathbf{p}(i)]_{(k)}$ the *parent class* of $[i]_{(k+1)}$.

We partition $E \setminus E(\mathbb{T})$ into $\mathcal{A}_{Ret}(\mathbb{T}) \uplus \mathcal{C}_{Ret}(\mathbb{T})$. Let $0 \leq k \leq l$, $j \in L_k$, $i \in L_l$ and $e := (i, j) \in E \setminus E(\mathbb{T})$. Then $e \in \mathcal{C}_{Ret}(\mathbb{T})$ iff one of the mutually exclusive conditions (56) holds:

$$[j]_{(k)} \notin P([o]_{(0)}, [i]_{(l)}), \quad (56a)$$

$$l \geq 2 \wedge [j]_{(k)} \in P([o]_{(0)}, [\mathbf{p}(\mathbf{p}(i))]_{(l-2)}) \wedge \xi_i \neq \xi_j, \quad (56b)$$

$$l \geq 2 \wedge [j]_{(k)} \in P([o]_{(0)}, [\mathbf{p}(\mathbf{p}(i))]_{(l-2)}) \wedge \xi_i = \xi_j \wedge s(C) = \mathbf{S}, \quad (56c)$$

where $C \in P([j]_{(k)}, [\mathbf{p}(i)]_{(l-1)})$ the unique class with $\mathbf{p}(C) = [j]_{(k)}$,

$$l \geq 1 \wedge [j]_{(k)} = [\mathbf{p}(i)]_{(l-1)} \wedge \xi_i \neq \xi_j \wedge s(i) = \mathbf{D} \wedge j < \mathbf{p}(i), \quad (56d)$$

$$l \geq 1 \wedge [j]_{(k)} = [\mathbf{p}(i)]_{(l-1)} \wedge \xi_i \neq \xi_j \wedge s(i) = \mathbf{S}, \quad (56e)$$

$$l \geq 1 \wedge [j]_{(k)} = [\mathbf{p}(i)]_{(l-1)} \wedge \xi_i = \xi_j \wedge s(i) = \mathbf{S} \wedge j < \mathbf{p}(i). \quad (56f)$$

And $e \in \mathcal{A}_{Ret}(\mathbb{T})$ iff one of the mutually exclusive conditions (57) holds:

$$[j]_{(k)} = [i]_{(l)}, \quad (57a)$$

$$l \geq 2 \wedge [j]_{(k)} \in P([o]_{(0)}, [\mathbf{p}(\mathbf{p}(i))]_{(l-2)}) \wedge \xi_i = \xi_j \wedge s(C) = \mathbf{D}, \quad (57b)$$

where $C \in P([j]_{(k)}, [\mathbf{p}(i)]_{(l-1)})$ the unique class with $\mathbf{p}(C) = [j]_{(k)}$,

$$l \geq 1 \wedge [j]_{(k)} = \mathbf{p}([i]_{(l)}) \wedge \xi_i \neq \xi_j \wedge s(i) = \mathbf{D} \wedge j > \mathbf{p}(i), \quad (57c)$$

$$l \geq 1 \wedge [j]_{(k)} = \mathbf{p}([i]_{(l)}) \wedge \xi_i = \xi_j \wedge s(i) = \mathbf{D}, \quad (57d)$$

$$l \geq 1 \wedge [j]_{(k)} = \mathbf{p}([i]_{(l)}) \wedge \xi_i = \xi_j \wedge s(i) = \mathbf{S} \wedge j > \mathbf{p}(i). \quad (57e)$$

Remark. Of particular importance are the *deep edges* in (57b). This is where we use the particular structure of $G(\vec{\xi})$. Paths in the tree returning to a previously visited polymer find here always an admissible edge to add, thus excluding the tree from $\mathcal{T}_{Ret}(G(\vec{\xi}))$.

Proposition 25. *The map*

$$Ret : \mathcal{T}_G \rightarrow \mathcal{C}_G \quad \mathbb{T} \mapsto Ret(\mathbb{T}) := (I, E(\mathbb{T}) \uplus \mathcal{A}_{Ret}(\mathbb{T})) \quad (58)$$

is a partition scheme of G with $[\mathbb{T}, Ret(\mathbb{T})] = \mathcal{E}_{Ret}^{-1}(\mathbb{T})$.

Proof. If we admit that the partition in algorithm 24 satisfies the compatibility condition (47), then proposition 25 is a direct consequence of proposition 16. Thus we show (47) for \mathcal{E}_{Ret} and $\mathcal{A}_{Ret}(\mathbb{T})$.

Fix $\mathbb{T} \in \mathcal{T}_G$ and $H \in \mathcal{E}_{Ret}^{-1}(\mathbb{T})$. Let $0 \leq k \leq l$, $j \in L_k$, $i \in L_l$ and $e := (i, j) \in E \setminus E(\mathbb{T})$. Let $(H_n)_{n \in \mathbb{N}_0}$ and $(T_n)_{n \in \mathbb{N}_0}$ be the sequences associated with H from algorithm 22. For $\emptyset \neq F \subseteq E \setminus E(H)$ set $\tilde{H} := (I, E(H) \uplus F)$ and let $(\tilde{H}_n)_{n \in \mathbb{N}_0}$ and $(\tilde{T}_n)_{n \in \mathbb{N}_0}$ be its associated sequences from algorithm 22.

We define the *influence level* $m(e)$ of e as the unique solution of $[j]_{(k)} \wedge [i]_{(l)} \subseteq L_{m(e)}$. We claim that for each $N \in \mathbb{N}$ (compare with (65)):

$$(\forall e \in F : m(e) \geq N) \Rightarrow (H_n|_{T_n})_{n=0}^N = (\tilde{H}_n|_{\tilde{T}_n})_{n=0}^N. \quad (59)$$

To show (59) we proceed by induction over n , for $n \in [N]_0$. By definition $H_0|_{T_0} = \tilde{H}_0|_{\tilde{T}_0}$. For the induction step from $n < N$ to $n + 1$ we show that algorithm 22 is not influenced by the presence of such an $e \in F$. The addition of e does not change \tilde{P}_n nor the s classification of its vertices compared to P_n . Let i and j be the ancestors of i and j at level $n + 1$ of \mathbb{T} respectively. Then they are both in P_n and \tilde{P}_n . As $[i]_{(n+1)} = [j]_{(n+1)}$ in \mathbb{T} we have two possibilities in $H_n|_{U_n}$: both i and j are classified \mathbf{S} and in an \mathbf{S} connected component of $H_n|_{U_n}$ or both i and j are classified \mathbf{D} and in a \mathbf{D} connected component of $H_n|_{U_n}$. In both cases the presence of e in \tilde{H} could merge the connected components of i and j in $H_n|_{U_n}$ respectively into one connected component of $\tilde{H}_n|_{\tilde{U}_n}$, but only of the same classification. Therefore all vertices in $\tilde{P}_n = P_n$ end in connected components of $H_n|_{U_n}$ and $\tilde{H}_n|_{\tilde{U}_n}$ of the same classification respectively. Thus $S_n = \tilde{S}_n$ and $T_n = \tilde{T}_n$. Finally the selection of the parent in (rbs) and (rbd) is independent of $H_n|_{U_n}$ and $\tilde{H}_n|_{\tilde{U}_n}$ in all possible combinations. We conclude that $H_{n+1}|_{T_{n+1}} = \tilde{H}_{n+1}|_{\tilde{T}_{n+1}}$.

Observe that if $e \in \mathcal{A}_{Ret}(\mathbb{T})$, then by (57) e has influence level k . To show (47a) we assume that $F \subseteq \mathcal{A}_{Ret}(\mathbb{T})$. If e is of type (57a), then it is removed

during iteration $(k - 1)$ by **(rcs)** or **(rcd)**. If e is of type (57b), then it is removed by **(rid)** during iteration k . If e is of type (57c), then it is removed by **(rudd)** during iteration k . If e is of type (57e), then it is removed by **(rus)** during iteration k . If e is of type (57d), then it is removed by **(ruds)** during iteration k .

To show (47b) we assume that $F' := F \cap \mathcal{C}_{Pen}(\mathbb{T}) \neq \emptyset$. Choose $e \in F$ with $m(e) = N := \min \{m(f) : f \in F'\}$ minimal. We demonstrate that the presence of e causes $(H_n|_{T_n})_{n \in \mathbb{N}_0}$ to diverge from $(\tilde{H}_n|_{\tilde{T}_n})_{n \in \mathbb{N}_0}$ exactly at level $N+1$, that is (59) holds and $H_{N+1}|_{T_{N+1}} \neq \tilde{H}_{N+1}|_{\tilde{T}_{N+1}}$. We go through all the cases of (56):

Case e of type (56a): It is evident that $N < k \vee l$. Hence there exist ancestors \mathbf{i} and \mathbf{j} of i and j in L_{N+1} respectively with $[\mathbf{p}(\mathbf{i})]_{(N)} = [\mathbf{p}(\mathbf{j})]_{(N)} = [j]_{(k)} \wedge [i]_{(l)} \subseteq L_N$ ($i = \mathbf{i}$ iff $l = N$ possible. Same for j and \mathbf{j}). It also follows from (56a) that $[\mathbf{i}]_{(N+1)} \neq [\mathbf{j}]_{(N+1)}$. This means that during iteration N of algorithm 22, without loss of generality in that order, \mathbf{i} is classified as **S** in an **S** connected component of $H_N|_{U_N}$ and \mathbf{i} is classified as **D** in a **D** connected component of $H_N|_{U_N}$. The addition of e in \tilde{H} places \mathbf{i} and \mathbf{j} in the same connected component of $\tilde{H}_N|_{\tilde{U}_N}$, via the path $\mathbf{i} \leftrightarrow i \leftrightarrow j \leftrightarrow \mathbf{j}$. This means that \mathbf{i} is an **S** vertex in a **D** connected component of $\tilde{H}_N|_{\tilde{U}_N}$ and thus is not selected into \tilde{S}_N by **(rbd)**. Thus $T_{N+1} \neq \tilde{T}_{N+1}$.

Case e of type (56b): Here $N = k$. Let \mathbf{i} be the ancestor of i with $\mathbf{p}([\mathbf{i}]_{(N+1)}) = [j]_{(N)}$. As $\xi_i \neq \xi_j$ the addition of e in \tilde{H} classifies i as **D** in step N . Therefore $i \in \tilde{S}_N$ by **(rbd)**, but $i \notin T_N$. Thus $T_{N+1} \neq \tilde{T}_{N+1}$.

Case e of type (56c): Here $N = k$. Let \mathbf{i} be the ancestor of i with $\mathbf{p}([\mathbf{i}]_{(N+1)}) = [j]_{(N)}$. As $\xi_i = \xi_j$ the addition of e in \tilde{H} classifies i as **S** in step N . As $i \leftrightarrow \mathbf{i}$ in $H_N|_{U_N}$ and hence $\tilde{H}_N|_{\tilde{U}_N}$ we know that i is in a **D** connected component of $\tilde{H}_N|_{\tilde{U}_N}$, namely the one of \mathbf{i} . Therefore $i \in \tilde{S}_N$ by **(rbs)**, but $i \notin T_N$. Thus $T_{N+1} \neq \tilde{T}_{N+1}$.

Case e of type (56d): Here $N = k$. Let \mathbf{i} be the parent of i in $[j]_{(N)}$. The addition of e in \tilde{H} lets **(rpd)** select j to be the parent of i in $\tilde{T}_{N+1}|_{\tilde{T}_{N+1}}$. Thus $T_{N+1} \neq \tilde{T}_{N+1}$.

Case e of type (56e): Here $N = k$. Let \mathbf{i} be the parent of i in $[j]_{(N)}$. The addition of e in \tilde{H} classifies i as **D** during step N instead of **S**. Therefore its parent in $\tilde{T}_{N+1}|_{\tilde{T}_{N+1}}$ is chosen by **(rpd)** instead of **(rps)** and is not \mathbf{i} any more. Thus $T_{N+1} \neq \tilde{T}_{N+1}$.

Case e of type (56f): Here $N = k$. Let \mathbf{i} be the parent of i in $[j]_{(N)}$. The addition of e in \tilde{H} lets **(rps)** select j to be the parent of i in $\tilde{T}_{N+1}|_{\tilde{T}_{N+1}}$. Thus $T_{N+1} \neq \tilde{T}_{N+1}$. \square

Proposition 26 (Properties of $\mathcal{T}_{Ret}(G(\vec{\xi}))$). *Let $\mathbb{T} \in \mathcal{T}_{Ret}(G(\vec{\xi}))$ and let C_i be*

the set of children of i in \mathbb{T} . Then

$$|C_i| = |\text{supp } \vec{\xi}_{C_i}| \quad (60a)$$

$$(\text{supp } \vec{\xi}_{C_i}) \setminus \{\xi_i\} \text{ is an independent subset of } \mathcal{I}^*(\xi_i) \quad (60b)$$

$$\forall k \in \mathbb{N}_0, i \in L_k : \text{supp } \vec{\xi}_{[i]_{(k)}} \text{ is an independent subset of } \mathcal{P} \quad (60c)$$

$$\forall i \in I \setminus \{o\} : i \text{ is } \mathbf{D} \Rightarrow \xi_i \notin \text{supp } \vec{\xi}_{P(o, \mathbf{p}(i))}. \quad (60d)$$

Proof. Fix k and let $i, j \in L_{k+1}$ with $i \sim_{(k+1)} j$. If $\xi_i \approx \xi_j$, then $e := (i, j) \in E$ as $G = G(\vec{\xi})$ (6). Hence by (57a) $e \in E(\text{Ret } \mathbb{T})$ and thus $\text{Ret}(\mathbb{T}) \neq \mathbb{T}$. This shows (60c), which implies (60b), which in turn implies (60a).

Suppose there exists a vertex i violating (60d). If $\mathbf{p}(i) = o$ we have a direct contradiction to the \mathbf{D} classification of i . If $\mathbf{p}(i) \neq o$, then the violation implies the existence of $j, j \in P(o, \mathbf{p}(i))$ with $d_{\mathbb{T}}(o, j) + 1 = d_{\mathbb{T}}(o, i) < d_{\mathbb{T}}(o, i)$ and $\xi_i = \xi_j \neq \xi_j$. Take such a j minimal with respect to $d_{\mathbb{T}}(o, j)$. Consider the edge $e := (j, i)$, which is in E due to the fact that $G = G(\vec{\xi})$ (6). It is admissible with respect to \mathbb{T} of type (57b). Hence $e \in E(\text{Ret}(\mathbb{T}))$ and thus $\text{Ret}(\mathbb{T}) \neq \mathbb{T}$. \square

5.5 The synthetic scheme

The *synthetic scheme* Syn interpolates between the behaviour of the greedy scheme Pen in algorithm 17 and the returning scheme Ret in algorithm 22. The static information comprises the total order on I , a vector $\vec{g} \in \{\mathbf{G}, \mathbf{R}\}^{\mathcal{P}^*}$, the cluster structure of $G(\vec{\xi})$, with $\vec{\xi} \in \mathcal{P}^I$ and the choice of the root $o \in I$.

We only state the exploration algorithm. We omit the edge partition for reconstruction from a tree and the correctness proof, as they mirrors the one for the returning scheme in section 5.4, with greedy and returning classes taking the role of same and different classes respectively. These greedy and returning classes are encoded by \vec{g} : the greedy class contains all children with the same polymer label or with $g_{(\xi_v, \xi_{\mathbf{p}(v)})} = \mathbf{G}$, while the returning class those with $g_{(\xi_v, \xi_{\mathbf{p}(v)})} = \mathbf{R}$.

Algorithm 27 ($Syn(\vec{g})$ exploration). Let $H \in \mathcal{C}_G$. For every k , let H_k, T_k, U_k, B_k and P_k be as in algorithm 13. The missing parts to construct H_{k+1} from H_k are:

Call an edge $(i, j) \in E(C \cap P_k, B_k) \cap E(H)$ *greedy* (or \mathbf{G}) iff $b_{\xi_i, \xi_j} = \mathbf{G}$ and *returning* (or \mathbf{R}) iff $b_{\xi_i, \xi_j} = \mathbf{R}$. Likewise call a vertex $i \in P_k$ same iff all such (i, j) are greedy and returning iff there exists such a non-same (i, j) . Finally we say that a connected component C of $H_k|_{U_k}$ is greedy iff all vertices in $C \cap P_k$ are greedy and returning iff $C \cap P_k$ contains at least one returning vertex.

If C is an \mathbf{G} connected component of $H_k|_{U_k}$:

(sbs) SELECT $C \cap S_k := C \cap P_k$.

(sis) As $C \cap I_k = \emptyset$ REMOVE nothing.

(sps) For $i \in C \cap S_k$ let $j_i := \text{argmin} \{j \in B_k : (i, j) \in E(H_k)\}$. SELECT (i, j_i) .

(sus) For $i \in C \cap S_k$ REMOVE all $(i, j) \in E(H_k)$ with $j_i \neq j \in B_k$.

(scs) REMOVE all of $E(C \cap S_k) \cap E(H_k)$.

If C is a \mathbf{R} connected component of $H_k|_{U_k}$:

(sbd) SELECT $C \cap S_k := \{i \in C \cap P_k : i \text{ is } \mathbf{R}\}$.

(sid) $C \cap I_k = \{i \in C \cap P_k : i \text{ is } \mathbf{G}\}$. REMOVE all of $E(B_k, (C \cap I_k)) \cap E(H_k)$.

(spd) For $i \in C \cap S_k$ let $j_i := \operatorname{argmin} \{j \in B_k : (i, j) \in E(H_k) \text{ is } \mathbf{R}\}$. SELECT (i, j_i) .

(sudd) For $i \in C \cap S_k$ REMOVE every $\mathbf{R} (i, j) \in E(H_k)$ with $j_i \neq j \in B_k$.

(suds) For $i \in C \cap S_k$ REMOVE every $\mathbf{G} (i, j) \in E(C \cap S_k, B_k) \cap E(H_k)$.

(scd) REMOVE all of $E(C \cap S_k) \cap E(H_k)$.

5.6 On the impossibility of globally excluding a fixed neighbour

The holy grail would be a scheme excluding a globally fixed neighbour of each vertex. This is impossible, though. The counterexample is a polymer system (\mathcal{P}, \approx) isomorph (ignoring loops) to a large circle of size N . Take the cluster formed by $\vec{\xi} \in \mathcal{P}^N$ with $\operatorname{supp} \vec{\xi} = \mathcal{P}$, which is again isomorph to the circle of size N . It has N spanning trees and only one of them can be expanded to the full circle. This means, that every partition scheme has $N - 1$ singleton trees on $G(\vec{\xi})$. Fix the root and the globally forbidden neighbours. Then every finite family approximation not returning to forbidden neighbours contains at most one of those $N - 1$ trees. Hence no partition scheme with globally excluded neighbours exists.

6 Proof of the new SCUBs

This section contains the proofs of the new SCUBS (22),(23) and (27). We use the new partition schemes, which give us more information about their singleton trees to use in our tree-operators. To carry this extra information over between successive applications of the derived tree-operator, we work on a space labelled by an extension of \mathcal{P} with additional information. This is the multiplexing step. To obtain the SCUB we have project down onto a \mathcal{P} -indexed space, leading to the max in (22),(23) and (27).

We start with the returning SCUB (23) in section 6.1. Section 6.2 then proves the reduced SCUB (22) again, by showing that it is just a relaxation of the the tree-operator underlying the returning SCUB. The proof of the synthetic SCUB (27) does not use any new ideas beyond the ones present in the proof of the returning SCUB (23) in section 6.1. The notational load is much heavier, though, as everything is parametrised by \vec{g} . We therefore omit this proof.

6.1 The returning SCUB

In this section we prove the returning SCUB (23). The first part of the proof is the same as the one for the returning SCUB (22) in section 3. Thus we only have to deal with escaping pairs (Λ, γ) , that is pairs with $\mathcal{I}^*(\gamma) \setminus \Lambda \neq \emptyset$. Instead of the limit of the one polymer partition ratios $\varphi_\Lambda^\gamma(-\vec{\rho})$, we look at the *escaped pinned series*

$$\begin{aligned} \Psi_{(\gamma, \varepsilon)}^*(\vec{\rho}) &:= \rho_\gamma \lim_{\Lambda \nearrow \mathcal{P} \setminus \{\varepsilon\}} \frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(-\vec{\rho}) \\ &= \sum_{n \geq 0} \frac{1}{n!} \sum_{\vec{\xi} \in (\mathcal{P} \setminus \{\varepsilon\})^n} |u(\gamma, \xi_1, \dots, \xi_n)| \prod_{i=1}^n \rho_{\xi_i}. \end{aligned} \quad (61)$$

Bounding $\varphi_{\mathcal{P} \setminus \{\varepsilon\}}^\gamma(-\vec{\rho})$ from below or $\Psi_{(\gamma, \varepsilon)}^*(\vec{\rho})$ from above are equivalent (70). We show that if the returning SCUB (23) holds with non-strict inequality, then $\vec{\rho} < \vec{1}$ and

$$\forall (\gamma, \varepsilon) \in \mathcal{P}_* : \quad \Psi_{(\gamma, \varepsilon)}^*(\vec{\rho}) \leq \frac{\phi_\gamma^{\text{ret}}(\vec{\mu}) - \mu_\gamma}{1 - \rho_\gamma} < \infty. \quad (62)$$

Consequently $\vec{\rho} \in \mathcal{R}_\mathcal{P}$. Statement (62) is a consequence of an application of proposition 11 to a suitable tree-operator T and with Q being the escaping pinned series. This immediately implies that T has to live on a space indexed by \mathcal{P}_* . The rest of the proof consists of: applying the scheme *Ret* to bound the Ursell factors in the escaping pinned series, deriving the tree-operator T and showing that it satisfies the conditions of proposition 11.

Proof of (62). Let $\mathbb{T} \in \mathcal{T}_{\text{Ret}}(G(\vec{\xi}))$. Property (60d) is equivalent to:

$$\forall i \in I \setminus \{o\} : \nexists j, j \in P(o, \mathfrak{p}(i)) : \quad d_{\mathbb{T}}(o, j) < d_{\mathbb{T}}(o, i) \wedge \xi_i = \xi_j \neq \xi_j.$$

Therefore the polymer labels of $P(o, i)$ form a *lazy self-avoiding walk* on $\text{supp } \vec{\xi}$. In particular we can look at the ordered sequence of *avoided polymers* for $i \in I$. By (61) we only regard $\vec{\xi}$ with $\text{supp } \vec{\xi} \subseteq \mathcal{P} \setminus \{\varepsilon\}$. Hence the avoided polymers for i are a polymer-valued sequence starting with ε and adding ξ_j if we use a **D** edge after j on the path $P(o, i)$. The avoided polymers of o are (ε) and therefore the sequence is non-empty for every i . Call ε_i the last polymer in the avoided-polymer sequence of vertex i . We have $\xi_i \approx \varepsilon_i$ by construction for every $i \in I$. Hence $(\xi_i, \varepsilon_i)_{i \in I} \in \mathcal{P}_*^I$.

We focus on a vertex i and its children in \mathbb{T} . Property (60b) implies that their polymer labels form a compatible set. And property (60d) implies, that if we have an **S** i then $(\xi_i, \varepsilon_i) = (\xi_{\mathfrak{p}(i)}, \varepsilon_{\mathfrak{p}(i)})$, while if we have a **D** i then $\varepsilon_i = \xi_{\mathfrak{p}(i)}$. These constraints are determined by the extended labels $(\xi_i, \varepsilon_i)_{i \in I}$. Set $I := [n]_0$ with $o := n$. We drop all other constraints on \mathbb{T} , apply Penrose's identity (37)

and get

$$\begin{aligned}
& |\mathbf{u}(\vec{\xi})| \\
&= |\mathcal{T}_{Ret}(G(\vec{\xi}))| \\
&= \sum_{\tau \in \mathcal{T}_n} [\tau \in \mathcal{T}_{Ret}(G(\vec{\xi}))] \\
&\leq \sum_{\tau \in \mathcal{T}_n} \prod_{i \in [n]_0} c_{s_i}^{\text{mul}}((\xi_i, \varepsilon_i), (\xi_{i_1}, \varepsilon_{i_1}), \dots, (\xi_{i_{s_i}}, \varepsilon_{i_{s_i}})).
\end{aligned} \tag{63a}$$

where the $(s_i)_{i=0}^n$ denote the number of children of i in τ and

$$\begin{aligned}
& c_n^{\text{mul}}((\xi_0, \varepsilon_0), \dots, (\xi_n, \varepsilon_n)) \\
&:= \sum_{A \subseteq [n]} \left(\prod_{i \in A} [(\xi_i, \varepsilon_i) = (\xi_0, \varepsilon_0)] \prod_{i \neq j \in A} [\xi_j \not\approx \xi_i] \right) \\
&\quad \times \left(\prod_{i \in [n] \setminus A} [\xi_i \in \mathcal{I}^*(\xi_0) \setminus \{\varepsilon_0\}, \varepsilon_i = \xi_0] \prod_{i \neq j \in [n] \setminus A} [\xi_j \not\approx \xi_i] \right). \tag{63b}
\end{aligned}$$

The $(c_n^{\text{mul}})_{n \in \mathbb{N}_0}$ are the tree-invariant functions of the labelled, rooted trees consisting of the root 0 and exactly n children.

Let $Y := [0, \infty]^{\mathcal{P}_*}$. Denote by i_{mul} the injection from X into Y , *multiplexing* values by ignoring the escape coordinate in \mathcal{P}_* . Define the operator $\phi^{\text{mul}} : Y \rightarrow Y$ by

$$\phi_{(\gamma, \varepsilon)}^{\text{mul}}(\vec{u}) := \sum_{n \geq 0} \frac{1}{n!} \sum_{(\vec{\xi}, \vec{\varepsilon}) \in \{(\gamma, \varepsilon)\} \times \mathcal{P}_*^n} c_n^{\text{mul}}(\vec{\xi}, \vec{\varepsilon}) \prod_{i=1}^n u_{(\xi_i, \varepsilon_i)}.$$

We see that $c_n^{\text{mul}}(\vec{\xi}, \vec{\varepsilon})$ is the coefficient of $\prod_{i=1}^n u_{(\xi_i, \varepsilon_i)}$ in the product of the following terms:

$$\begin{aligned}
& (1 + u_{(\gamma, \varepsilon)}) \\
&= \sum_{n \geq 0} \frac{1}{n!} \sum_{(\vec{\xi}, \vec{\varepsilon}) \in \{(\gamma, \varepsilon)\} \times \mathcal{P}_*^n} \prod_{i=1}^n [(\xi_i, \varepsilon_i) = (\gamma, \varepsilon)] \prod_{i \neq j=1}^n [\xi_j \not\approx \xi_i] \prod_{i=1}^n u_{(\xi_i, \varepsilon_i)}
\end{aligned}$$

and

$$\begin{aligned}
& \Xi_{\mathcal{I}^*(\gamma) \setminus \{\varepsilon\}}(\vec{u}_{\{(\xi, \gamma) : \xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}\}}) \\
&= \sum_{n \geq 0} \frac{1}{n!} \sum_{(\vec{\xi}, \vec{\varepsilon}) \in \{(\gamma, \varepsilon)\} \times \mathcal{P}_*^n} \prod_{i=1}^n [\xi_i \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}, \varepsilon_i = \gamma] \prod_{i \neq j=1}^n [\xi_j \not\approx \xi_i] \prod_{i=1}^n u_{(\xi_i, \varepsilon_i)}.
\end{aligned}$$

Therefore

$$\phi_{(\gamma, \varepsilon)}^{\text{mul}}(\vec{u}) = (1 + u_{(\gamma, \varepsilon)}) \Xi_{\mathcal{I}^*(\gamma) \setminus \{\varepsilon\}}(\vec{u}_{\{(\xi, \gamma) : \xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}\}}).$$

For $\vec{r} \in Y$, define the tree-operator

$$T_{\vec{r}} : Y \rightarrow Y \quad \vec{u} \mapsto \vec{r} \phi^{\text{mul}}(\vec{u}).$$

Using the fact that

$$\forall \gamma \in \mathcal{P} : \quad \phi_\gamma^{\text{ret}}(\vec{\mu}) = \max \{ \phi_{(\gamma, \varepsilon)}^{\text{mul}}(i_{\text{mul}}(\vec{\mu})) : \varepsilon \in \mathcal{I}^*(\gamma) \},$$

we deduce from (23) that

$$T_{i_{\text{mul}}(\vec{\rho})}(i_{\text{mul}}(\vec{\mu})) \leq i_{\text{mul}}(\vec{\mu}).$$

We apply proposition 10, for $k = 1$, to $T_{i_{\text{mul}}(\vec{\rho})}$ and get a finite series fixpoint $R(i_{\text{mul}}(\vec{\rho})) \leq i_{\text{mul}}(\vec{\mu})$. Then (63a) implies that

$$\forall (\gamma, \varepsilon) \in \mathcal{P}_* : \quad \rho_\gamma \Psi_{(\gamma, \varepsilon)}^*(\vec{\rho}) \leq R_{(\gamma, \varepsilon)}(i_{\text{mul}}(\vec{\rho})) \leq \mu_\gamma.$$

For every $(\gamma, \varepsilon) \in \mathcal{P}_*$, $T_{i_{\text{mul}}(\vec{\rho})}$ has to count the terms $|\mathbf{u}(\gamma)| = 1$ and $|\mathbf{u}(\gamma, \gamma)| = 1$, with weights $i_{\text{mul}}\vec{\rho}_{(\gamma, \varepsilon)} = \rho_\gamma$ and $\rho_\gamma \mu_\gamma$ respectively. Therefore $(T_{i_{\text{mul}}(\vec{\rho})})_{(\gamma, \varepsilon)} \geq \rho_{(\gamma, \varepsilon)}(1 + \mu_{(\gamma, \varepsilon)})$. We met the conditions of proposition 11 and (62) follows. □

6.2 The reduced SCUB

It is evident that (23) is stronger than (22), by the inequality $\phi^{\text{ret}}(\vec{\mu}) \leq \phi^{\text{red}}(\vec{\mu})$. Although we already have proven (22) in section 3 by an inductive proof based on the fundamental identity, we want to point out that $\phi^{\text{red}}(\vec{\mu})$ comes from a tree-operator, too. If we relax (63b) to

$$\begin{aligned} & c_n^{\text{mul}}((\xi_0, \varepsilon_0), \dots, (\xi_n, \varepsilon_n)) \\ & \leq \sum_{A \subseteq [n]} \left(\prod_{i \in A} [(\xi_i, \varepsilon_i) = (\xi_0, \varepsilon_0)] \right) \left(\prod_{i \in [n] \setminus A} [\xi_i \in \mathcal{I}^*(\xi_0) \setminus \{\varepsilon_0\}, \varepsilon_i = \xi_0] \right), \end{aligned}$$

then we see that $c_n^{\text{mul}}(\vec{\xi}, \vec{\varepsilon})$ is the coefficient of $\prod_{i=1}^n u_{(\xi_i, \varepsilon_i)}$ in the product of the terms $(1 + u_{(\gamma, \varepsilon)})$ and $\prod_{\xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}} (1 + u_{(\xi, \gamma)})$. We thus have

$$\phi_{(\gamma, \varepsilon)}^{\text{mul}}(\vec{u}) \leq (1 + u_{(\gamma, \varepsilon)}) \prod_{\xi \in \mathcal{I}^*(\gamma) \setminus \{\varepsilon\}} (1 + u_{(\xi, \gamma)}).$$

Finishing the proof of (62) with the preceding inequality, corresponding to a relaxed tree-operator on Y , we naturally arrive at (22).

7 Epilogue

7.1 The universal minimality of Kotecký & Preiss' SCUB

It has already been shown in [FP07] that Kotecký & Preiss' SCUB (20a) also stems from a tree-operator. We just want to point out that this tree-operator ignores the choice of partition scheme in Penrose's identity 8. It only uses the structure of a cluster, as inherited from its support in the polymer system (see figure 5). This makes it a universal relaxation and common denominator to every conceivable SCUB.

7.2 Further improvements

This section assumes the reader to be familiar with section 5. We outline some improvements to the current SCUBs, which may be of interest if one one wants to get computational bounds and is not satisfied by the simple SCUBs presented yet.

The first, and most straightforward, improvement is to use higher-depth tree-operators. By cutting the trees in depth k pieces one can extract more restrictions on the trees. The same holds for the second improvement, namely multiplexing onto spaces indexed by bigger sets than \mathcal{P}_* . This transfers even more information between successive applications of the tree-operator.

A third improvement is to bring more information from the polymer system into the exploration algorithm. One way to so is to choose the parent of a selected vertex also by its polymer label. Fix a collection $\{<_\gamma: \gamma \in \mathcal{P}\}$ of total orders $<_\gamma$ on $\mathcal{I}(\gamma)$. The parent selection step then is:

(gp): For $i \in C \cap S_k$ let $A_C^i := \{j \in B_k : (i, j) \in E(H_k)\}$. Order A_C^i totally via

$$j <_{A_C^i} j \Leftrightarrow (\xi_j <_{\xi_i} \xi_j) \vee (\xi_j = \xi_j \wedge j < j) . \quad (64)$$

Let $j_i := \min \{j \in A_C^i\}$ with respect to $<_{A_C^i}$. **SELECT** (i, j_i) .

This excludes certain vertices on the previous tree level of a vertex to having an admissible edge to this vertex. Thus it demands tree-operators of depth 2 or higher to take effect. See [Tem12, section 5.5.4] for further details.

Finally, one could imagine basing the selection of new vertices on a fixed number of previously selected levels and/or peaking a fixed depth ahead into the yet unexplored part of H .

8 Acknowledgements

I am grateful to Roberto Fernández for the time he took to explain me his work and encourage my attempts at extending it. The visits at the University of Utrecht have been supported by the RGLIS short visit grants 4076 and 4446 from the European Science Foundation (ESF). This work has been also supported by the Austrian Science Fund (FWF), project W1230-N13.

9 Appendix: Proof of proposition 20

Proof. If we admit that the partition in algorithm 19 satisfies the compatibility condition (47), then proposition 20 is a direct consequence of proposition 16. Thus we show (47) for \mathcal{E}_{Pen} and $\mathcal{A}_{Pen}(\mathbb{T})$.

Fix $\mathbb{T} \in \mathcal{T}_G$ and $H \in \mathcal{E}_{Ret}^{-1}(\mathbb{T})$. Let $0 \leq k \leq l$, $j \in L_k$, $i \in L_l$ and $e := (i, j) \in E \setminus E(\mathbb{T})$. Let $(H_n)_{n \in \mathbb{N}_0}$ and $(T_n)_{n \in \mathbb{N}_0}$ be the sequences associated with H from algorithm 22. For $\emptyset \neq F \subseteq E \setminus E(H)$ set $\tilde{H} := (I, E(H) \uplus F)$ and let $(\tilde{H}_n)_{n \in \mathbb{N}_0}$ and $(\tilde{T}_n)_{n \in \mathbb{N}_0}$ be its associated sequences from algorithm 22.

For $e \in F$ let $m(e)$ be the level of $i \wedge j$. We claim that for each $N \in \mathbb{N}$:

$$(\forall e \in F : m(e) \geq N) \Rightarrow (H_n|_{T_n})_{n=0}^N = (\tilde{H}_n|_{\tilde{T}_n})_{n=0}^N. \quad (65)$$

We show (65) by induction over n . By definition $H_0|_{T_0} = \tilde{H}_0|_{\tilde{T}_0}$. For the induction step from $n < N$ to $n+1$ we show that algorithm 17 is not influenced by the presence of such an $e \in F$. The presence of e does not change \tilde{P}_n compared to P_n in **(pb)**.

Observe that if $e \in \mathcal{A}_{Ret}(\mathbb{T})$, then by (50) $m(e) = k$. To show (47a) we assume that $F \subseteq \mathcal{A}_{Ret}(\mathbb{T})$. If e is of type (50a), then it is removed during iteration $(k-1)$ by **(pc)**. If e is of type (50b), then it is removed by **(pu)** during iteration k .

To show (47b) we assume that $F' := F \cap \mathcal{C}_{Pen}(\mathbb{T}) \neq \emptyset$. Choose $e \in F$ with $m(e) = N := \min \{m(f) : f \in F'\}$. We demonstrate that the presence of e causes $(H_n|_{T_n})_{n \in \mathbb{N}_0}$ to diverge from $(\tilde{H}_n|_{\tilde{T}_n})_{n \in \mathbb{N}_0}$ exactly at level $N+1$, that is (65) holds and $H_{N+1}|_{T_{N+1}} \neq \tilde{H}_{N+1}|_{\tilde{T}_{N+1}}$. We go through all the cases of (49):

Case e of type (49a): Here $N = k$. The presence of e lets **(pb)** SELECT $i \in \tilde{P}_k$.

Case e of type (49b): Here $N = k$. The presence of e lets **(pp)** SELECT i as the parent of i in \tilde{T}_{N+1} instead of $\mathfrak{p}(i)$. \square

10 Appendix: Pinned connected function vs one polymer partition ratios

The relations in this section are either to interpreted formally or if a SCUB holds. The pinned connected function is a product of one polymer partition ratios [SS05, (3.8)]:

$$\frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(\vec{z}) = \frac{\Xi_{\Lambda \setminus \mathcal{I}(\gamma)}(\vec{z})}{\Xi_\Lambda(\vec{z})} = \frac{1}{\varphi_\Lambda^\gamma(\vec{z})} \prod_{i=1}^m \frac{1}{\varphi_{\Lambda \setminus \{\gamma, \xi_1, \dots, \xi_{i-1}\}}^{\xi_i}(\vec{z})}, \quad (66)$$

where $\{\xi_1, \dots, \xi_m\} := \Lambda \cap \mathcal{I}^*(\gamma)$. On the other hand, the logarithm of the reduced correlations is an integral over the pinned connected function [BFPS11, (A.3)]:

$$\log \varphi_\Lambda^\gamma(\vec{z}) = z_\gamma \int_0^1 \frac{\partial \log \Xi_\Lambda}{\partial z_\gamma}(\vec{z}(\alpha)) d\alpha \quad (67)$$

with

$$\vec{z}(\alpha) := \begin{cases} z_\xi & \xi \neq \gamma \\ \alpha z_\gamma & \xi = \gamma. \end{cases}$$

Taking the limit $\Lambda \nearrow \mathcal{P}$, we have the following relations between the pinned series and the one polymer partition ratios in the classic case:

$$\Psi_\gamma(\vec{\rho}) \leq \frac{1}{\varphi_{\mathcal{P}}^\gamma(-\vec{\rho})} \prod_{\xi \in \mathcal{I}^*(\gamma)} \frac{1}{\varphi_{\mathcal{P}}^{\xi_i}(-\vec{\rho})}, \quad (68)$$

Thus the finiteness of $\Psi(\vec{\rho})$ is equivalent to the positivity of $\varphi_{\mathcal{P}}$. The converse relation follows from (67):

$$\varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) \geq \exp(-\rho_{\gamma} \Psi_{\gamma}(\vec{\rho})) . \quad (69)$$

In the escaping case we have

$$\Psi_{(\gamma, \varepsilon)}^*(i_{\text{mul}}(\vec{\rho})) \leq \frac{1}{\varphi_{\mathcal{P} \setminus \{\varepsilon\}}^{\gamma}(-\vec{\rho})} \prod_{\xi \in \mathcal{I}^*(\gamma)} \frac{1}{\varphi_{\mathcal{P} \setminus \{\gamma\}}^{\xi_i}(-\vec{\rho})} \quad (70)$$

and

$$\varphi_{\mathcal{P} \setminus \{\varepsilon\}}^{\gamma}(-\vec{\rho}) \geq \exp\left(-\rho_{\gamma} \Psi_{(\gamma, \varepsilon)}^*(i_{\text{mul}}(\vec{\rho}))\right) . \quad (71)$$

The relationship between classic and escaping quantities is given by the following inequalities and comparisons. The pinned series is exactly

$$\Psi_{\gamma}(\vec{\rho}) = \frac{1}{\varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho})} \prod_{\xi \in \mathcal{I}^*(\gamma)} \frac{1}{\varphi_{\mathcal{P} \setminus \{\gamma\}}^{\xi_i}(-\vec{\rho})} . \quad (72)$$

The one polymer partition ratios compare as

$$\varphi_{\mathcal{P}}^{\gamma}(-\vec{\rho}) = 1 - \frac{\rho_{\gamma}}{\prod_{i=1}^m \varphi_{\mathcal{P} \setminus \{\gamma, \xi_{i+1}, \dots, \xi_m\}}^{\xi_i}(-\vec{\rho})} \geq 1 - \frac{\rho_{\gamma}}{\prod_{i=1}^m \varphi_{\mathcal{P} \setminus \{\gamma\}}^{\xi_i}(-\vec{\rho})} , \quad (73)$$

where $\{\xi_1, \dots, \xi_m\} := \mathcal{I}^*(\gamma)$. The pinned series fulfil the identity

$$\Psi_{\gamma}(\vec{\rho}) = \left(1 + \rho_{\gamma} \Psi_{\gamma}(\vec{\rho})\right) \Xi_{\mathcal{I}^*(\gamma)}\left(i_{\text{mul}}(\vec{\rho}) \Psi_{(\cdot, \gamma)}^*(i_{\text{mul}}(\vec{\rho}))\right) . \quad (74)$$

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